Comments on the distorted-wave Born-approximation cross sections for the 2^1P excitation of He†

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The cross sections for the $2\,^1P$ excitation of He by electron impact have been calculated with the distorted-wave Born approximation (by Madison and Shelton) and with the plane-wave Born approximation (by Kim and Inokuti). Although the distorted-wave description of the incident electron results in greatly improved cross sections at large angles compared to the plane-wave method, this paper points out that a substantial part [(35–80)%] of the difference in the two methods for small-angle scattering comes from using different He wave functions in the two computations.

Recently, Madison and Shelton[1] calculated the cross sections for the electron-impact excitation of He from its ground state to the $2\,^1P$ state by use of the distorted-wave Born approximation (DWBA) and showed that their values are in much better agreement with the angular distribution measured by Chamberlain *et al.*[2] than are those by Kim and Inokuti[3] calculated with the plane-wave Born approximation (PWBA). The purpose of this Comment is to show that a substantial part of the improvement indicated in that comparison comes from the different He wave functions used in Refs. 1 and 3.

In the PWBA, the incident electron before and after the collision is described by plane waves of appropriate momenta, and the indistinguishability of the incident electron from those in the target atom (the exchange effect) is often ignored as was done in Ref. 3. Furthermore, the Coulomb interaction between the incident electron and the atom is treated as a first-order perturbation.

In the DWBA, the incident electron is described by continuum wave functions obtained by solving the one-electron Schrödinger equation in the field created by the static charge distribution of the atom. The repulsion between the incident electron and the atomic electrons is treated as in the PWBA, while the Coulomb interaction with the (screened) nucleus has been fully incorporated in the distorted waves for the incident electron. Furthermore, Madison and Shelton[1] included the exchange effect by antisymmetrizing the total wave function for the colliding system. Neither the PWBA nor the DWBA takes account of the distortion of the charge distribution of the atom, and the wave functions for the initial and final states of the (isolated) atom explicitly enter the formulation of both methods. The numerical values of the cross sections therefore depend on the choice of wave functions for the atom in both approximations.

The numerical results for the DWBA in Ref. 1 were obtained by using the Hartree-Fock (HF) wave functions, whereas those for the PWBA in

TABLE I. Comparison of experiment with the distorted-wave (DW) and the plane-wave (PW) Born cross sections for the 2^1P excitations of He by electron impact.

Incident energy (eV)	Deflection angle (deg)	Experiment (Ref. 2)	Electron-impact cross sections (a.u.) Hartree-Fock DW(Ref. 1)	Hartree-Fock PW(Present)	Correlated PW(Ref. 3)
100	5	2.411	2.892	3.292	3.507
	10	0.918	1.176	1.287	1.367
	15	0.335	0.459	0.489	0.516
	20	0.123	0.179	0.189	0.198
200	5	2.911	3.113	3.308	3.523
	10	0.563	0.647	0.664	0.703
	15	0.124	0.152	0.155	0.162
300	5	2.339	2.404	2.487	2.647
	7.5	0.821	0.876	0.894	0.947
	10	0.312	0.347	0.351	0.369

TABLE II. Ratios of the 2^1P excitation cross sections at different angles.

Incident energy (eV)	Angles in the ratio	Experiment (Ref. 7)	Electron-impact cross-section ratios Hartree-Fock DW(Ref. 1)	Hartree-Fock PW(Present)	Correlated PW(Ref. 3)
100	10°/5°	0.381	0.407	0.391	0.390
	15°/5°	0.139	0.159	0.149	0.147
	20°/5°	0.0510	0.0619	0.0574	0.0565
200	10°/5°	0.193	0.208	0.201	0.200
	15°/5°	0.0426	0.0488	0.0469	0.0460
300	7.5°/5°	0.351	0.364	0.359	0.358
	10°/5°	0.133	0.144	0.141	0.139

Ref. 3 were obtained from the correlated wave functions by Weiss.[4] The Weiss wave functions consist of over 50 terms of Hylleraas-type variables and, for most applications, their quality is comparable to that of the wave functions by Pekeris and Schiff.[5]

It is true that the DWBA should produce more reliable cross sections than the PWBA in principle, provided that the uncertainties in the wave functions of the atom are reduced substantially. Understandably, the numerical procedure for the DWBA is far more involved than that for the PWBA, and no DWBA calculations with the Weiss wave functions or with others of comparable complexity have been done so far.

Quantitative study of the advantages and merits of the DWBA over the PWBA should therefore be based on a comparison between the numerical results obtained with the same wave functions, rather than with wave functions of substantially different qualities as was done in Ref. 1.

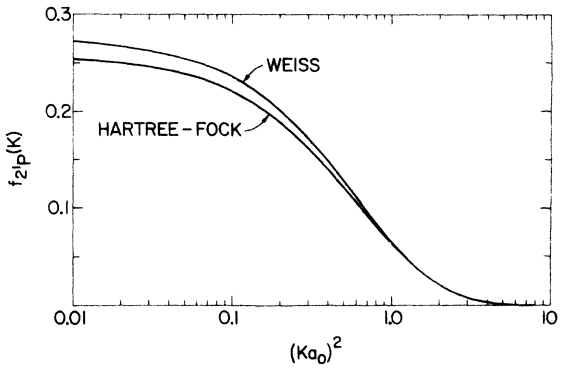

FIG. 1. Generalized oscillator strength $f_{2^1P}(K)$ for the 2^1P excitation of He as a function of the magnitude of the momentum transfer K in atomic units (a_0 = Bohr radius). The upper curve was calculated from the Weiss wave functions (Ref. 3), and the lower from the Hartree-Fock wave functions. The almost complete merging of the two curves beyond $(Ka_0)^2 \approx 2$ indicates that the two types of wave functions correspond to similar charge distributions in the core region of He.

In Table I, the PWBA cross sections calculated with the same HF wave functions[6] as those used in Ref. 1 are compared with the DWBA results. For the incident electron energy of 300 eV, it is clear that (65–80)% of the "improvements" of the DWBA cross section over the PWBA cross sections calculated with the correlated Weiss wave functions really come from the different wave functions. Even at 100-eV incident energy, the DWBA results are closer to the PWBA results from the HF wave functions than they are to the experimental values.

Moreover, the experimental angular distribution in Ref. 2 was obtained by determining the absolute cross sections at a 5° scattering angle, then using the ratios at larger angles *relative* to the 5° data, as determined earlier by Vriens *et al.*[7] When we compare the ratios of cross sections at various angles to those at 5° (Table II), the PWBA results with the Weiss wave functions show the best agreement with the experimental ratios.

Of course, such a comparison *does not* imply that the PWBA is intrinsically better than the DWBA. On the contrary, the DBWA has definite advantages over the PWBA, e.g., for scattering at large angles ($\gtrsim 30°$), as is demonstrated clearly by many graphs on large-angle scattering in Ref. 1. The interaction of the incident electron with the nucleus is a major factor for the large-angle

TABLE III. Dipole oscillator strengths for the 2^1P excitation of He.

Wave functions	Oscillator strength Length form	Velocity form
Schiff and Pekeris	0.2762	0.2762
Weiss	0.2759	0.2761
Hartree-Fock (This work)	0.2583	0.2402

scattering, and the PWBA is likely to fail badly in this case because nuclear scattering is excluded in the PWBA. On the other hand, the DWBA still has its own shortcomings, such as the neglect of the distortion of the charge distribution of the atom as the incident electron passes by the target. The numerical results in Table II simply show that for cases in which both the PWBA and the DWBA give reasonable answers, the advantages of the latter method can easily be masked by the use of less-accurate wave functions as was done in Ref. 1.

Incidentally, many papers on the PWBA cross sections for the $2\,^1P$ excitations[8] have been published, but none of them were calculated from the HF wave functions for both the initial and final states of He. Since it is more likely that cross sections from theories more advanced than the PWBA would be calculated with the HF wave functions rather than with those similar to the Weiss wave functions, some PWBA results from the HF wave functions are presented in Fig. 1 and Table III. As is well known, the PWBA results for arbitrary incident energy and scattering angle can be computed easily once the generalized oscillator strength for the excitation is known as a function of the momentum transferred during the collision.[9] The generalized oscillator strength calculated from the HF wave functions is presented in Fig. 1 and compared with that from the Weiss wave function in the length form.[3] The generalized oscillator strength reduces to the dipole-oscillator strength in the limit of zero momentum transfer. The dipole-oscillator strengths, by the length and velocity formulas from the HF wave functions, are compared with those from correlated wave functions in Table III. The experimental excitation energy[10] (21.221 eV) was used for both the generalized and dipole-oscillator strengths calculated from the HF wave functions. As expected from the lower cross sections from the HF wave functions (Table I), the dipole-oscillator strength is also smaller than that calculated from the correlated wave functions.

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[6]The Hartree-Fock wave functions were calculated from a computer program written by C. Froese-Fischer [Comput. Phys. Commun. 1, 151 (1970)] but partly modified by P. S. Bagus. Full self-consistency was required for both the core and valence orbitals of the $2\,^1P$ wave function, corresponding to the relaxed-core case in Ref. 1.

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[8]See, for instance, references cited by S. P. Ojha, P. Tiwari, and D. K. Rai, Can. J. Phys. 50, 2253 (1972), and also those in Refs. 1 and 3.

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