

Correlation in time-dependent density-functional-theory studies of antiproton-helium collisions

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Correlation effects are examined in the context of time-dependent density-functional-theory calculations of antiproton-helium collisions. An approximation for the correlation potential as well as two models for the correlation integral are explored. The first of these makes use of frozen correlation, while the second is appropriated from the world of laser-induced ionization. Total cross sections for both single and double ionization in the impact energy range 5–2000 keV are presented. While the results of the first model provide little improvement over an independent electron model description the second model agrees quite well with experimental results for both single and double ionization. Our results also lend credence to the belief that an appropriate approximation of the correlation integral is more important in reproducing correlation effects than the correlation potential.

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I. INTRODUCTION

Atomic collision systems, while interesting in their own right, are often considered as a means of investigating general features of quantum dynamical processes. An important example is the antiproton-helium collision system. This system is often chosen for its relative simplicity. As the helium atom contains only two electrons and one nuclear center it is, perhaps, the most basic multibody configuration one might consider. The presence of a negatively charged impact ion removes the necessity of considering charge-transfer processes. This means that the analysis may focus on single and double ionization (as well as the possibility of target excitation). In addition, as long as impact energies remain above 1 keV a precise quantum-mechanical description of both target and projectile is of little importance [1,2]. This allows one to make use of the semiclassical approximation where the projectile is described in terms of a time-dependent Coulomb potential rather than a quantum particle. The simplicity of this system makes it an ideal candidate for the investigation of theoretical many-body techniques, as one may include complicated electron correlation effects without the time-dependent Schrödinger equation (TDSE) becoming intractable.

The existence of experimental data [3–6] for the antiproton-helium system helps to guide theoretical calculations. As one might expect, the most successful calculations are those that attempt to directly solve the TDSE. Borrowing the nomenclature of the recent antiproton collision review article [1] we will refer to such calculations as correlated two-electron calculations. For our purposes the most interesting are those which produce both single and double ionization [7–9]. Antiproton-helium calculations can also be performed using effective single-particle descriptions. Included in this class are those calculations which employ both one active electron (e.g., [10,11]), which can only describe single ionization, and independent electron model [12–15] techniques.

Time-dependent density-functional theory [16] (TDDFT) is one such effective single-particle scheme which can be

used to incorporate electron correlation. In TDDFT electron correlation enters by two distinct processes: first, through the exchange-correlation potential, which encodes the many-body interactions of a system such that the exact one-particle density may be determined by solving a set of single-particle equations; second, in the context of TDDFT all observables are expressible as functionals of the one-particle density. Depending upon how these functionals are approximated they include varying degrees of correlation. This ranges from no correlation (independent electron model descriptions) to varying degrees of approximate correlation [17–20].

Using the aforementioned antiproton-helium collision system as a test bed we examine the effects of correlation on single and double ionization within the context of TDDFT. This investigation will precede through the application of two models for the so-called correlation integral, that is, correlation in the observable functionals, as well as one model for the correlation potential. Both the first model for the correlation integral and our approximate correlation potential will make use of frozen correlation, an idea that was first introduced into the world of atomic collisions by Martín and Salin [21,22] and was later used by others to analyze double ionization [23]. The second model is adapted from the world of laser-induced ionization and was originally considered by Wilken and Bauer [18]. The difference between the results produced by these models and those of an independent electron model will help shed light on the role of both types of correlation in single and double ionization processes.

Our discussion will begin in Sec. II A with a brief introduction to the foundations of TDDFT. This will be followed in Sec. II B by a discussion of the observable problem in TDDFT. In the subsequent sections we will describe the practical aspects of our calculations. This will consist of the selection of an appropriate ground-state approximation for the helium atom (Sec. II C1), a description of a procedure for generating radial functions compatible with a given ground state as well as an approximation for the correlation potential (Sec. II C2), and a description of our dynamical calculations (Sec. II D). In Sec. III we present and discuss the results of our calculations. Finally our conclusions are offered in Sec. IV. Atomic units are used unless stated otherwise.

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II. THEORY

A. The Runge-Gross theorem

A system of N interacting particles is described by an N -particle wave function $\Psi(t)$ that evolves via the TDSE

$$i \frac{d\Psi(t)}{dt} = \hat{H}(t)\Psi(t). \quad (1)$$

The Hamiltonian \hat{H} can be written

$$\hat{H}(t) = \hat{T} + \hat{V}_{ee} + \hat{V}_{\text{ext}}(t), \quad (2)$$

where \hat{T} is the kinetic energy, \hat{V}_{ee} is the interelectron potential, and $\hat{V}_{\text{ext}}(t)$ is an external single-particle potential.

For a fixed potential \hat{V}_{ee} the Runge-Gross theorem [24], which forms the basis of TDDFT, establishes a one-to-one correspondence between the potential $\hat{V}_{\text{ext}}(t)$ and the one-particle density

$$n(\mathbf{r}_1, t) = N \sum_{\mathbf{s}} \int d^3 r_2 \dots d^3 r_N |\Psi(\mathbf{x}_i, t)|^2, \quad (3)$$

where $\mathbf{x}_i = (\mathbf{r}_i, s_i)$ labels the position and spin of the i th particle. We say that the external potential is a functional of the one-particle density $\hat{V}_{\text{ext}}(t) = \hat{V}_{\text{ext}}[n](t)$. It should be noted that the mapping provided by the Runge-Gross theorem defines the external potential only up to an arbitrary time-dependent function. This time-dependent function translates into a time-dependent phase factor in the wave function and as such will not enter into quantities of physical interest [16].

In practice the correspondence is used to map a system described by an interacting many-body TDSE onto a system of noninteracting particles represented by the orbitals $\varphi_i(\mathbf{r}, t)$. If we define the noninteracting system such that it reproduces the exact interacting one-particle density

$$n(\mathbf{r}, t) = \sum_{i=1}^N |\varphi_i(\mathbf{r}, t)|^2, \quad (4)$$

the Runge-Gross theorem guarantees the existence of a unique multiplicative potential $v_{\text{KS}}[n]$ which determines the orbitals φ_i via

$$i \frac{\partial}{\partial t} \varphi_i(\mathbf{r}, t) = \left(-\frac{\Delta}{2} + v_{\text{KS}}[n](\mathbf{r}, t) \right) \varphi_i(\mathbf{r}, t), \quad (5)$$

with $i = 1, \dots, N$.

These equations are known as the time-dependent Kohn-Sham (TDKS) equations and the potential, $v_{\text{KS}}[n](\mathbf{r}, t)$, the Kohn-Sham potential. This potential can be decomposed into

$$v_{\text{KS}} = v_{\text{ext}} + v_{\text{H}} + v_{\text{xc}}, \quad (6)$$

where v_{ext} is the external potential, v_{H} is the Hartree screening potential, and v_{xc} is the exchange-correlation (xc) potential which encodes the (nonclassical) interelectron interactions. Both the xc potential and the Hartree potential will be uniquely determined by the one-particle density, that is, they are both functionals of n ($v_{\text{xc}}[n]$ and $v_{\text{H}}[n]$). Formally v_{ext} is also a functional of the density, however in the present situation the form of v_{ext} is determined by the nuclear and projectile potentials (see Sec. IID). It is often convenient to split v_{xc} into

an exchange and a correlation part,

$$v_{\text{xc}}[n] = v_{\text{x}}[n] + v_{\text{c}}[n]. \quad (7)$$

While this mapping is, in theory, exact, the precise functional relation between density and potential is not known. The xc potential must be approximated.

B. Observables

It can be shown that the Runge-Gross theorem also establishes a correspondence between the one-particle density and the value of any observable. Exact functionals for the determination of observables are known in only a handful of cases [25]. Much like the xc potential, the unknown functionals are usually approximated.

One case where the exact density functional is known is the average number of electrons released to the continuum, the so-called net ionization. For the case of the antiproton-helium collision system this is given by

$$p_{\text{net}}(t) = 2 - \int_T n(\mathbf{r}, t) d^3 r, \quad (8)$$

where T is some volume containing the target as well as all bound-state contributions to n [26]. The net ionization can be used to define the average probability for ionizing an electron,

$$p = \frac{1}{2} p_{\text{net}}. \quad (9)$$

With these definitions we can write the exact i -fold ($i = 0, 1, 2$) ionization probabilities [17],

$$p_0 = \frac{1}{2} \iint_T d^3 r_1 d^3 r_2 \rho(\mathbf{r}_1, \mathbf{r}_2, t_f), \quad (10)$$

$$p_1 = \int_T \int_{\mathbb{R}^3 \setminus T} d^3 r_1 d^3 r_2 \rho(\mathbf{r}_1, \mathbf{r}_2, t_f), \quad (11)$$

$$p_2 = \frac{1}{2} \iint_{\mathbb{R}^3 \setminus T} d^3 r_1 d^3 r_2 \rho(\mathbf{r}_1, \mathbf{r}_2, t_f), \quad (12)$$

where $\rho = 2|\psi|^2$ is the exact two-particle density at some final time t_f chosen large enough to ensure that the results do not vary for $t \geq t_f$ (see Sec. IID), as

$$p_0 = (1 - p)^2 + \frac{1}{2} I_c, \quad (13a)$$

$$p_1 = 2p(1 - p) - I_c, \quad (13b)$$

$$p_2 = p^2 + \frac{1}{2} I_c. \quad (13c)$$

The quantity I_c is referred to as the correlation integral [18] and is defined to be

$$I_c = \iint_T d^3 r_1 d^3 r_2 \left[\frac{\rho(\mathbf{r}_1, \mathbf{r}_2, t_f)}{n(\mathbf{r}_1, t_f)n(\mathbf{r}_2, t_f)} - \frac{1}{2} \right] n(\mathbf{r}_1, t_f) n(\mathbf{r}_2, t_f). \quad (14)$$

The simplest way to approximate a many-body system is by ignoring the interparticle interactions. Such models are known as independent electron models (IEMs). In analogy to this

we may calculate the ionization probabilities using an IEM description by ignoring I_c :

$$p_0^{\text{IEM}} = (1 - p)^2, \quad (15a)$$

$$p_1^{\text{IEM}} = 2p(1 - p), \quad (15b)$$

$$p_2^{\text{IEM}} = p^2. \quad (15c)$$

Obviously these simple binomial relations are consistent with the assumption of independent electrons.

As noted above, correlation enters TDDFT calculations both through observables (i.e., the ionization probabilities discussed in this section) and through the correlation potential. These two mechanisms may be treated independently. This means that one can apply Eq. (II B) to densities calculated using a scheme that includes any amount of correlation.

In the context of TDDFT we have no explicit knowledge of the two-particle density. Thus, if we wish to include correlation in the ionization probabilities we must approximate I_c . Models of this type have been used previously to describe ionization in laser interactions [17]. It was later shown that these models contain a pathology which forces them to essentially reproduce IEM results [27] (i.e., to use our notation $I_c \approx 0$). More recently Wilken and Bauer (WB) proposed a model for one-dimensional laser interactions that avoided these issues [18]. A vastly simplified version of this model has been applied to antiproton-helium collisions [19]. In this work we extend those previous accounts and evaluate I_c in the WB model without dimensional or other restrictions.

In the WB model the densities at time t_f in the first factor of Eq. (14) are approximated by the adiabatic densities

$$\begin{aligned} n^A(t_f) &= \begin{cases} [1 - N(t_f)]n_0 + N(t_f)n_1, & 0 \leq N(t_f) \leq 1, \\ [2 - N(t_f)]n_1 + [N(t_f) - 1]n_2, & 1 \leq N(t_f) \leq 2, \end{cases} \end{aligned} \quad (16)$$

and

$$\begin{aligned} \rho^A(t_f) &= \begin{cases} [1 - N(t_f)]\rho_0 + N(t_f)\rho_1, & 0 \leq N(t_f) \leq 1, \\ [2 - N(t_f)]\rho_1 + [N(t_f) - 1]\rho_2, & 1 \leq N(t_f) \leq 2, \end{cases} \end{aligned} \quad (17)$$

where

$$N(t_f) = \int_T d^3r n(\mathbf{r}, t_f) \quad (18)$$

is the number of bound electrons at time t_f [which can be expressed in terms of p as $N = 2(1 - p)$] and n_i and ρ_i are the i -electron one- and two-particle ground-state densities respectively. In this model the densities appearing in the first factor of the correlation integral are approximated by means of a linear interpolation between the ionized and unionized atom. Due to the fact that $n_0 = \rho_0 = \rho_1 = 0$ the correlation integral will be reduced to $I_c = -2(1 - p)^2$ for $0 \leq N(t_f) \leq 1$. This translates to $p_0 = 0$ resulting in a split between single and double ionization [for $N(t_f) = 1$ we have $p_1 = 1$ and $p_2 = 0$ while for $N(t_f) = 0$ $p_1 = 0$ and $p_2 = 1$].

In addition to the IEM and WB models we will also introduce a third model for the determination of ionization

probabilities in the context of TDDFT. The idea behind this model is to freeze the first factor of Eq. (14) in the ground state,

$$I_c = \iint_T \left[\frac{\rho_{\text{gs}}(\mathbf{r}_1, \mathbf{r}_2)}{n_{\text{gs}}(\mathbf{r}_1)n_{\text{gs}}(\mathbf{r}_2)} - \frac{1}{2} \right] n(\mathbf{r}_1, t_f) n(\mathbf{r}_2, t_f) d^3r_1 d^3r_2. \quad (19)$$

We will refer to this model as the frozen correlation model (FCM). An approximation of this kind may be justifiable for impact energies $E \geq 200$ keV where dynamic correlation effects are, arguably, less important [28]. The actual forms of the various densities appearing in Eq. (19) will be the focus of the next section.

C. Practical considerations

1. Ground-state approximations

Both WB and FCM require knowledge of the ground-state two-particle density ρ_{gs} of helium. To help facilitate calculations it is convenient to consider wave functions of the form

$$\psi_{\text{gs}}(\mathbf{r}_1, \mathbf{r}_2) = \sum_i C_i T_i(\mathbf{r}_1, \mathbf{r}_2), \quad (20a)$$

$$T_i(\mathbf{r}_1, \mathbf{r}_2) = R_{n_1 l_1}^{\text{gs}}(r_1) R_{n_2 l_2}^{\text{gs}}(r_2) Y_{l_1}^{m_1}(\Omega_1) Y_{l_2}^{m_2}(\Omega_2), \quad (20b)$$

with $C_i \in \mathbb{R}$ and $\Omega = (\theta, \phi) \in S^2$. The exchange-only optimized potential method (OPM) [29] can be used to generate a simple uncorrelated helium ground state [30],

$$\psi_{\text{gs}}(\mathbf{r}_1, \mathbf{r}_2) = R_{10}^{\text{gs}}(r_1) R_{10}^{\text{gs}}(r_2) Y_0^0(\Omega_1) Y_0^0(\Omega_2). \quad (21)$$

For the sake of consistency such an approximation should only be used when considering the IEM for the calculation of single and double ionization probabilities.

Slightly more complex approximations having the form of (II C1) can be found in the work of Silverman *et al.* [31]. In this paper two correlated helium ground-state approximations consisting of $1s1s'$ and $1s1s' + 2p^2$ (full) configurations are presented. The $1s1s'$ term refers to a Hylleraas-Eckart [32,33] type configuration which is a symmetrized sum of radially different $1s$ type orbitals. These wave functions are often used as simple models for electron correlation in the helium ground state in atomic collision calculations, e.g., [34] (see also the discussion in [35]).

If we require more accurate correlation the multiconfiguration Hartree-Fock method (MCHF) [36] is well suited to generating wave functions of the desired form. An approximation including all configurations of the form $ns-ms$ with $m, n \in \{1, 2, 3, 4\}$ (i.e., radial correlation only) will capture 41% of the correlation energy while a wave function that contains all allowed configurations from $1s^2$ to $4d^2$ will capture 97% of the correlation energy [37]. A list of the ground-state energies of these approximations can be found in Table I.

2. Excited orbitals and effective potentials

The helium ground state is a spin singlet. Due to this fact the two Kohn-Sham orbitals will be identical. We can then write

$$\varphi_1 = \varphi_2 = \varphi. \quad (22)$$

TABLE I. Energies of ground-state approximations for helium given in Hartree. OPM values from [29], values for the Silverman wave functions presented in [31], All MCHF values calculated using [38].

Wave function	Energy (a.u.)
OPM	-2.8617
Silverman $1s1s'$	-2.8756614
MCHF $1s-4s$	-2.878990082
Silverman full	-2.8952278
MCHF $1s-4d$	-2.902523084

We can expand n_T , the bound part of the one-particle density, in terms of the eigenfunctions of the initial Hamiltonian

$$n_T(\mathbf{r}, t) = 2|\varphi_T(\mathbf{r}, t)|^2, \quad (23)$$

$$\varphi_T(\mathbf{r}, t) = \sum_{n,l,m} a_{nlm}(t) R_{nl}(r) Y_l^m(\Omega), \quad (24)$$

where the amplitudes $a_{nlm}(t)$ are determined by solving the TDKS equation (Sec. IID). We wish to make use of radial functions (R_{nl}) which are compatible with our choice of ground-state approximation (R_{nl}^{gs}). In order to generate such functions we must first determine the effective potential which will reproduce a given ground-state approximation.

If we are given an approximation for the ground-state two-particle density (e.g., one discussed in the previous section) we may determine the ground-state one-particle density

$$n_{\text{gs}}(\mathbf{r}) = \int d^3r' \rho_{\text{gs}}(\mathbf{r}, \mathbf{r}') \quad (25)$$

($\rho_{\text{gs}} = 2|\psi_{\text{gs}}|^2$). We can define a real ground-state Kohn-Sham orbital by

$$n_{\text{gs}}(\mathbf{r}) = 2\varphi^{\text{gs}}(\mathbf{r})^2. \quad (26)$$

This orbital will satisfy a stationary equation

$$-\frac{\Delta}{2}\varphi^{\text{gs}}(\mathbf{r}) + v_{\text{eff}}(r)\varphi^{\text{gs}}(\mathbf{r}) = \epsilon_0\varphi^{\text{gs}}(\mathbf{r}) \quad (27)$$

with eigenvalue ϵ_0 for some potential v_{eff} . This equation can be solved for the potential

$$v_{\text{eff}}(r) = \frac{\Delta\varphi^{\text{gs}}(\mathbf{r})}{2\varphi^{\text{gs}}(\mathbf{r})} + \epsilon_0. \quad (28)$$

The eigenvalue can be fixed using the boundary condition $\lim_{r \rightarrow \infty} v_{\text{eff}}(r) = 0$ which implies that

$$\epsilon_0 = -\lim_{r \rightarrow \infty} \frac{\Delta\varphi^{\text{gs}}(\mathbf{r})}{2\varphi^{\text{gs}}(\mathbf{r})}. \quad (29)$$

By performing this operation on the ground-state approximations discussed in Sec. IIC1 we can determine the ground-state Kohn-Sham potentials associated with these densities. These effective potentials may be used to approximate v_{xc} (see Sec. IID).

Plotted in Fig. 1 are the differences of the effective potentials of the various ground-state approximations of Sec. IIC1 from the exact ground-state Kohn-Sham potential [39]. The results of the MCHF $1s-4d$ approximation are in

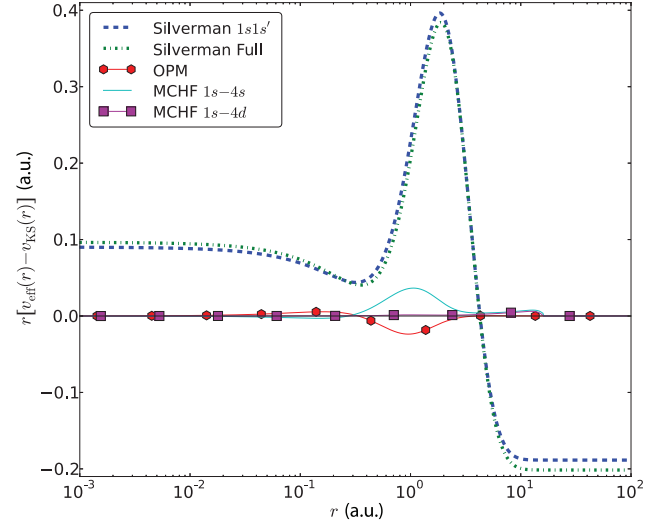


FIG. 1. (Color online) Comparison of the effective potentials of the various ground-state approximations for He.

good agreement with the exact potential. The $1s-4s$ wave function, that includes only radial correlation, also offers fine agreement outside of the bump centered around 1 a.u. where it overestimates the correlation potential. The OPM potential also differs in this region as it contains no correlation. Due to the fact that the MCHF routine [38] only produces data up to a radial distance of approximately 20 a.u. the Coulomb tail must be grafted onto the results of Eq. (28). This results in the slight irregularity evident in both MCHF potentials in this region.

The effective potentials obtained from the Silverman wave functions, on the other hand, capture neither the proper high or low r limit while at the same time wildly exaggerating the exact potential. In short, it would seem that the Silverman wave functions do a rather poor job of realistically modeling the local behavior of the helium ground state. When used in the WB and FCM versions of the correlation integral the densities obtained from the Silverman wave functions produce single and double ionization results which deviate significantly from those obtained from the other ground-state approximations (and experiment). Therefore, they will not be discussed in Sec. III. These facts may draw into question the use of these approximations for helium in quantum dynamical situations.

D. Dynamics

The final piece required to perform a full calculation is the time-dependent one-particle density $n(\mathbf{r}, t)$. This function will be determined by solving the TDKS equations (5) for the case of an antiproton-helium collision in the framework of the semiclassical approximation.

Specializing to this case the external potential becomes

$$v_{\text{ext}}(\mathbf{r}, t) = -\frac{2}{r} + \frac{1}{|\mathbf{r} - \mathbf{R}(t)|}, \quad (30)$$

where $\mathbf{R}(t) = (b, 0, vt)$ is the classical straight-line trajectory of the projectile with impact parameter (distance of closest approach) b and velocity v . If we ignore relativistic effects this results in an impact energy $E = 1/2m_{\bar{p}}v^2$. It should be noted that in the context of the calculation time is parametrized

such that the antiproton is initially located at $(b, 0, -45)$. In the final state of the calculation the antiproton is at $(b, 0, 45)$.

In the case of a two-electron spin-singlet system we can write the exchange potential exactly as

$$v_x = -\frac{1}{2}v_H. \quad (31)$$

The exchange and Hartree potentials can now be combined into one object,

$$v_{Hx} = \frac{1}{2} \int d^3r' \frac{n(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|}. \quad (32)$$

For ease we will split the Kohn-Sham potential into a time-dependent part $v(t)$ and a time-independent part v_0 . The potential v_0 will be the effective ground-state potential generated using the method of Sec. II C 2. In the case of the OPM ground state this includes the nuclear potential as well as the exact ground-state exchange and Hartree screening potentials. For the MCHF ground states v_0 will also include the (nearly exact) ground-state correlation potential. In either case the time-dependent potential $v(t)$ will contain the projectile potential as well as the time-dependent Hartree-exchange potential, i.e., we neglect time-dependent correlation. The TDKS equations can now be written as

$$i \frac{\partial}{\partial t} \varphi(\mathbf{r}, t) = \left(-\frac{\Delta}{2} + v_0 + v(t) \right) \varphi(\mathbf{r}, t). \quad (33)$$

This equation was solved using the basis generator method (BGM) [40] by expanding the time-dependent orbitals in terms of the basis functions

$$\varphi_{nlm}^K(\mathbf{r}) = W_T(r, \epsilon_T)^K \varphi_{nlm}^0(\mathbf{r}), \quad (34)$$

where

$$W_T(\mathbf{r}, \epsilon_T) = \frac{1 - e^{-\epsilon_T r}}{r}, \quad (35)$$

$\epsilon_T = 1$ is a regularizer and $\{\varphi_{nlm}^0\}$ are a set of eigenstates of the initial (in this case Kohn-Sham ground-state helium) Hamiltonian,

$$\varphi_{nlm}^0 = R_{nl}(r) Y_l^m(\Omega). \quad (36)$$

For the actual calculations we have used the same basis sets and parameters as in Ref. [15] (radial functions replaced with those determined in Sec. II C 2), i.e., when employing an exchange-only OPM ground state the calculation is identical to the one performed in [15].

III. RESULTS AND DISCUSSION

The calculations described in the previous section were carried out using both the OPM and the MCHF $1s-4d$ helium ground-state approximations. The ionization probabilities were determined using either Eq. (15) in the case of the IEM or Eq. (13) with the appropriate model for I_c in the case of the WB and FCM. From these probabilities the total cross sections for single and double ionization were calculated using

$$\sigma_i = \int p_i(\mathbf{b}) d^2b = 2\pi \int b p_i(b) db \quad (37)$$

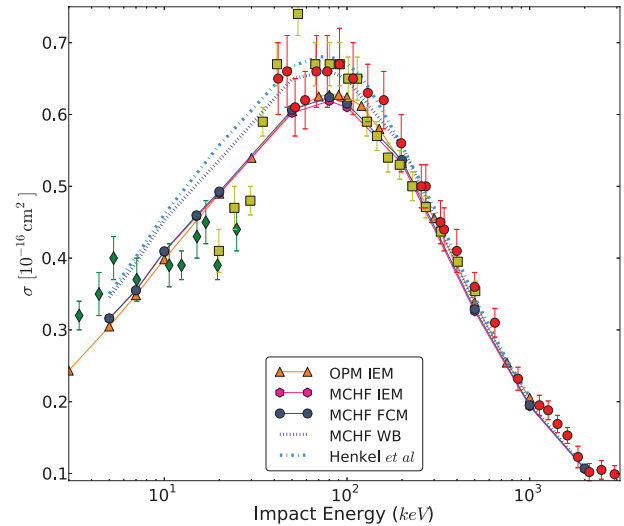


FIG. 2. (Color online) Calculated total cross section for single ionization of helium by antiproton impact compared to Henkel *et al.* [19] and experiment: \blacklozenge [5], \blacksquare [4], \bullet [3]. The results of MCHF IEM and MCHF FCM are on top of each other except in the region around the maximum.

($i = 1, 2$). The results of these calculations are presented in Figs. 2 and 3 where they are compared with the simplified WB model (sWB) of Henkel *et al.* [19]. In the following discussion we will refer to our calculations using a combination of two acronyms. The first acronym will denote the ground-state approximation used (OPM or MCHF for the MCHF $1s-4d$ configuration). The second acronym will refer to the model used for the correlation integral (IEM, FCM, or WB).

For the case of single ionization (Fig. 2) all of the models are in good agreement with the experimental data for impact energies larger than 50 keV. In addition, they all essentially coincide for very large impact energies. As impact energies decrease, the differences between the models become more

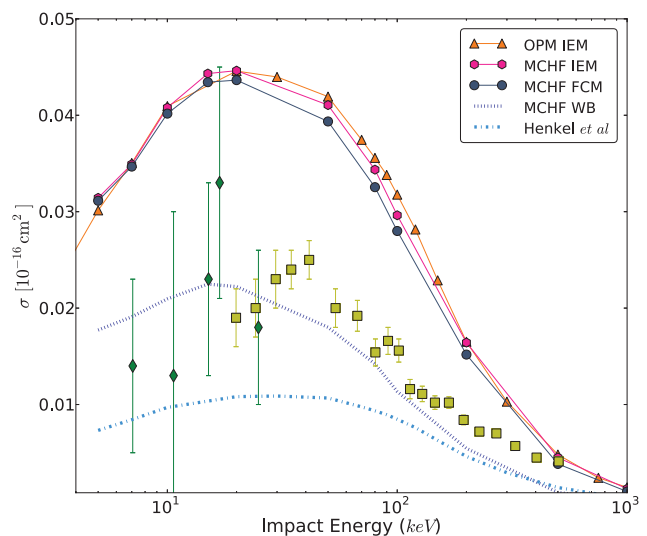


FIG. 3. (Color online) Calculated total cross section for double ionization of helium by antiproton impact compared to Henkel *et al.* [19] and experiment: \blacklozenge [6], \blacksquare [4].

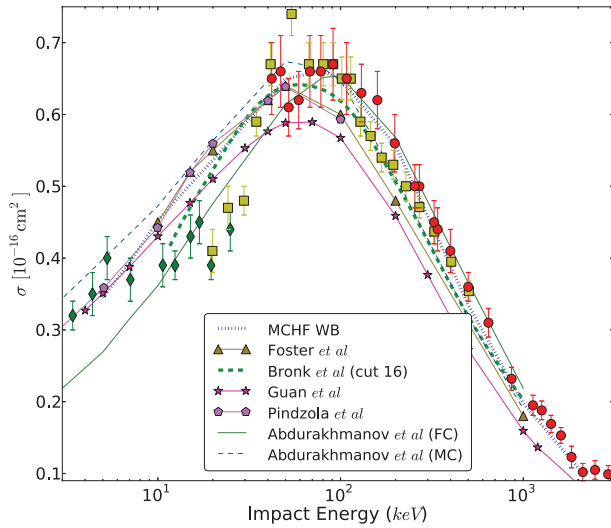


FIG. 4. (Color online) Comparison of the WB single ionization data to previous calculations: Foster *et al.* [8], Bronk *et al.* [7], Guan and Bartschat [9], Pindzola *et al.* [41], and Abdurakhmanov *et al.* [42] as well as experiment: \blacklozenge [5], \blacksquare [4], \bullet [3].

apparent. Near the maximum of the experimental data around 100 keV the WB model tends towards the higher range of the data while the IEM and FCM models tend towards the lower. The latter models do a better job of matching the drop in the data that takes place around 40 keV. The implementation of the full WB model provides only a slight reduction in the total cross section of the sWB.

The differences between these models become more apparent when considering double ionization. In this case the WB is a clear improvement over the sWB. The OPM IEM, MCHF IEM, and MCHF FCM models overstate double ionization at all but the highest impact energies.

The figures demonstrate little difference between the OPM IEM, MCHF IEM, and MCHF FCM results. In Fig. 3 we can see that the MCHF IEM slightly reduces the results of the OPM IEM. The MCHF FCM offers a further reduction. The only difference between the OPM IEM and MCHF IEM models is the inclusion of an approximate v_c , albeit one that in the latter case neglects time-dependent correlation.

When these results are compared to those of the WB model it lends credence to the belief that a good model for I_c is more important than v_c for obtaining accurate results [19]. While our v_c approximation ignores dynamic correlation an examination of the WB double ionization results suggests that a fully time-dependent correlation potential can serve only to fine tune results. In this instance dynamic correlation might increase double ionization at high impact energies while decreasing it at low.

Figures 4 and 5 present comparisons of the MCHF WB calculation with several previous calculations. Of the calculations chosen all produce both single and double ionization results except for Pindzola *et al.* [41] and Abdurakhmanov *et al.* [42], both of which use a close-coupling method. While Pindzola *et al.* reported results for both one- and two-active electrons only the latter will be considered. Abdurakhmanov *et al.* also produced two sets of data. Both data sets describe

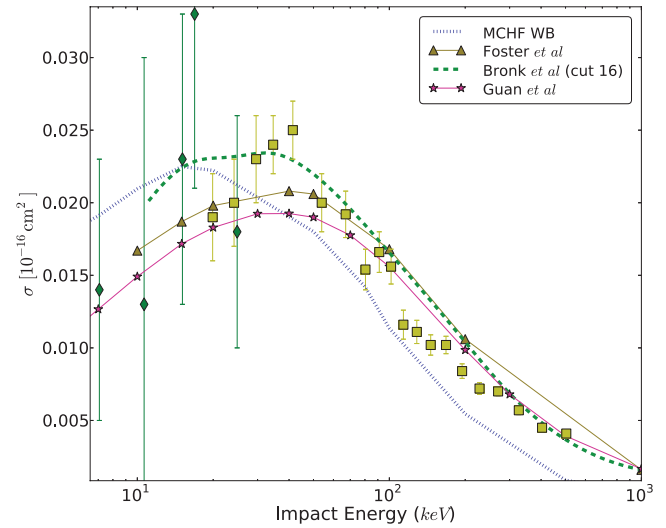


FIG. 5. (Color online) Comparison of the WB double ionization data to previous calculations: Foster *et al.* [8], Bronk *et al.* [7], and Guan and Bartschat [9] as well as experiment: \blacklozenge [6], \blacksquare [4].

the target using a configuration interaction wave function [43]. The first set comes from the so-called frozen core (FC) model where the inner (unionized) electron is forced to occupy the $1s$ state of He^+ . In the second set, the multiconfiguration (MC) description, both electrons are allowed to occupy a number of single-particle states.

Despite the fact that neither Pindzola *et al.* nor Abdurakhmanov *et al.* produce double ionization results they are included as they represent the most recent theoretical antiproton-helium collision calculations and are the only ones not discussed in the review article [1]. All of the theoretical data shown in Figs. 4 and 5 come from correlated two-electron calculations.

It can be seen (Fig. 4) that below 50 keV the results of Foster *et al.*, Pindzola *et al.*, Abdurakhmanov MC, and the WB model are rather similar. Above this point the data produced by Foster *et al.* and by Guan and Bartschat begin to underestimate the experimental data. While the multicore results of Abdurakhmanov *et al.* do not have the same issues at high impact energies the results slightly overestimate the data at the lowest impact energies. The frozen-core model of Abdurakhmanov *et al.* does a better job of reproducing experiment around 20 keV at the expense of underestimating the data below 10 keV. While Guan and Bartschat underestimate experiment at higher impact energies they are in agreement with the WB below 30 keV. Overall it can be seen that the WB model produces excellent single ionization results.

Turning to the results of the double ionization calculations (Fig. 5) it can be seen that all of the correlated two-electron calculations produce excellent agreement with experiment. The results of the WB model stack up quite well especially when one considers the fact that most effective single-particle calculations overstate double ionization [1]. In fact the WB model offers some of the best combined single and double ionization results produced to date.

IV. CONCLUSIONS

Throughout this work we have applied several models to the antiproton-helium collision system in the context of time-dependent density-functional theory in an attempt to incorporate correlation effects. These effects have been included through both an approximation for the correlation potential as well as two models for the correlation integral. We have presented single and double ionization results over a range of impact energies. The first approximate I_c model, the Wilken and Bauer model, generates good agreement with experiment. The second of these models, the frozen correlation model, produces results that differ only slightly from an independent electron model, i.e., it does not seem to be a useful approximation of I_c .

As a result of the method used to generate our approximate correlation potential it was found that the ground-state approximations of Silverman *et al.* [31] do not properly model the local structure of the helium ground state even though the total energies (global property) seem to suggest the contrary. This fact should caution one against future use of these wave

functions as models of the correlated helium ground state in collision calculations. It may also cause one to question past results for single and double ionization that have made use of these approximations.

A comparison of the results of the frozen correlation and Wilken and Bauer models to those of an independent electron model supports the belief that the correlation integral is more important than the correlation potential for obtaining properly correlated results [19]. The question still remains whether this conclusion also applies to collision systems involving positively charged projectile ions, for which electron capture competes with ionization, and to true many-electron systems, that is, those containing more than two electrons. These questions will be addressed in future work.

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