Boundary conditions of the exact impulse wave function

M. S. Gravielle* and J. E. Miraglia
Instituto de Astronomía y Física del Espacio, Consejo Nacional de Investigaciones Científicas y Técnicas, Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina
(Received 4 June 1996)

The behavior of the exact impulse wave function is investigated at intermediate and high impact energies. Numerical details of the wave function and its perturbative potential are reported. We conclude that the impulse wave function does not tend to the proper Coulomb asymptotic limit. For electron capture, however, it is shown that the impulse wave function produces reliable probabilities even for intermediate velocities and symmetric collision systems. [S1050-2947(97)09601-7]

PACS number(s): 34.70.+e

The exact impulse wave function (ψ^I) has been largely employed with success in different theoretical methods for the calculation of inelastic cross sections at high impact energies [1–5]. In particular, for capture we have developed the eikonal impulse (EI) approximation [6], which is a distorted wave method making use of ψ_f^I in the final channel and the eikonal wave function (ψ_i^E) in the initial channel. Both wave functions do preserve the proper normalization, i.e., $\langle \psi_a^I | \psi_b^I \rangle = \langle \psi_a^E | \psi_b^E \rangle = \delta_{ab}$, which leads to conservation of probability. Further, ψ_i^E is known to satisfy the proper Coulomb boundary conditions (CBC). A large amount of symmetric and asymmetric collision systems were studied with the EI method in the intermediate and high energy regions, and the results were in all cases in accord with the available data [6].

In spite of the generalized use of ψ^I, its asymptotic behavior was first called into question by Belkić *et al* [7], and more recently by Dewangan and Eichler [8], who stressed that ψ^I is *not consistent with the CBC*. In this work we calculate the exact behavior of ψ_f^I and its perturbative potential, reporting numerical details. The study is restricted to the final channel for electron capture; its application to the other channels is straightforward. As in Ref. [8], the impact parameter formalism is used. The origin of the coordinate system is chosen to be at the target nucleus considered at rest. The classical movement of the projectile is defined by the straight line trajectory: $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$, where $\mathbf{R}(t) = \mathbf{r}_T - \mathbf{r}_P$ is the internuclear coordinate, $\mathbf{b}$ is the impact parameter, $\mathbf{v}$ is the projectile velocity, and $\mathbf{b}\cdot\mathbf{v} = 0$ (see Fig. 1). Atomic units are used.

In the impact parameter treatment ψ_f^I reads [8]

$$\psi_f^I(\mathbf{r}_P,t) = f_e(\mathbf{r}_P,t) \int \frac{d\mathbf{k}}{(2\pi)^{3/2}} \widetilde{\varphi}_f(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{r}_P) \times D^-(Z_T, \mathbf{v}+\mathbf{k}; \mathbf{r}_T), \quad (1)$$

where $f_e(\mathbf{r}_P,t) = \exp[i(\mathbf{v}\cdot\mathbf{r}_P + v^2 t/2 - \varepsilon_f t)]$, φ_f is the final bound state with energy ε_f, and the tilde indicates the Fourier transform. The Coulomb distortion D^- is given by

$$D^-(Z_T,\mathbf{k};\mathbf{r}) = N(a)\, {}_1F_1(-ia, 1; -ikr - i\mathbf{k}\cdot\mathbf{r}), \quad (2)$$

where $N(a) = \exp(\pi a/2)\Gamma(1+ia)$, $a = Z_T/k$, and Z_T is the target nuclear charge. From Eq. (1) the well-known continuum distorted wave (CDW) wave function

$$\psi_f^{\mathrm{CDW}}(\mathbf{r}_P,t) = f_e(\mathbf{r}_P,t)\varphi_f(\mathbf{r}_P) D^-(Z_T,\mathbf{v};\mathbf{r}_T) \quad (3)$$

can be derived by using the so-called peaking approximation, which is based on the argument that $\widetilde{\varphi}_f(\mathbf{k})$ has a sharp peak around $\mathbf{k} = \mathbf{0}$ [9]. Notice that ψ_f^{CDW} does satisfy the CBC, i.e., $\psi_f^{\mathrm{CDW}} \to \phi_f^{\infty}$ as $t \to +\infty$, being

$$\phi_f^{\infty}(\mathbf{r}_P,t) = f_e(\mathbf{r}_P,t)\varphi_f(\mathbf{r}_P)\exp[ia_T \ln\alpha(t)], \quad (4)$$

with $\alpha(t) = vR(t) + \mathbf{v}\cdot\mathbf{R}(t)$, and $a_T = Z_T/v$. One should also notice that ψ_f^{CDW} does *not* preserve the normalization, that is, $\langle \psi_a^{\mathrm{CDW}} | \psi_b^{\mathrm{CDW}} \rangle \neq \delta_{ab}$. The eikonal wave function ψ_f^{E} reads as Eq. (4) with $\beta(t) = vr_T + \mathbf{v}\cdot\mathbf{r}_T$ instead of $\alpha(t)$.

Since ψ_f^{CDW} can be obtained from ψ_f^I, and $\psi_f^{\mathrm{CDW}} \to \phi_f^{\infty}$ as $t \to +\infty$, we were led to believe that ψ_f^I also satisfied the CBC [6]. As pointed out by Belkić *et al.* [7] and Dewangan and Eichler [8], that is not true. This failure will be studied in detail in this work.

Unlike ψ_f^{CDW} the expression of ψ_f^I in terms of the impact parameter cannot be obtained in closed-form. We were so forced to calculate ψ_f^I by performing the 3D numerical integral involved in Eq. (1). The task is more complex than the evaluation of the corresponding T-matrix element due to the presence of the hypergeometric function ${}_1F_1$, which causes the integrand to oscillate greatly. The numerical error of the results was estimated to be less than 1%.

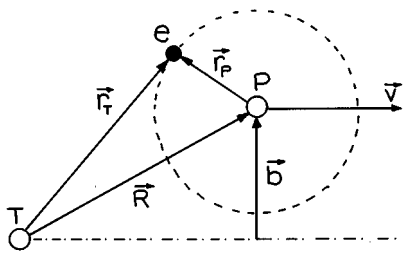

FIG. 1. Coordinate systems.

*Also at Departamento de Física, Universided Nacional de Buenos Aires, Buenos Aires, Argentina.

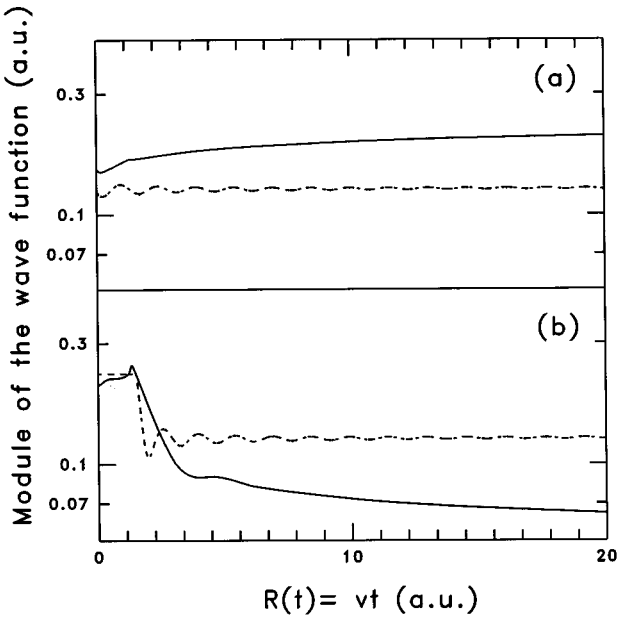

FIG. 2. Module of the final wave function for the case of impact parameter $\mathbf{b}=\mathbf{0}$ as a function of $R(t)=vt$ (in atomic units). The process considered is $H^+ + H(1s) \rightarrow H(1s) + H^+$ at $v=2$ a.u. Theories: solid line, $|\psi_f^I|$; dashed line, $|\psi_f^{\mathrm{CDW}}|$. The electronic coordinate is (a) $\mathbf{r}_P = r_0\hat{\mathbf{v}}$; (b) $\mathbf{r}_P = -r_0\hat{\mathbf{v}}$; with $r_0 = 1.5$ a.u.

We restrain our calculations to the simplest collisional system

$$H^+ + H(1s) \rightarrow H(1s) + H^+ \tag{5}$$

for $v=2$ a.u. This impact velocity corresponds to the lowest energy range (intermediate energies) for which the impulse hypothesis holds. Although the behavior of $\psi_f^I(\mathbf{r}_P,t)$ is here analyzed for the particular case $\mathbf{b}=\mathbf{0}$ in terms of $R(t)=vt$, the conclusions drawn below can be extended for other relevant impact parameters. The module of the electronic coordinate $\mathbf{r}_P$ is taken to be the value $r_0=1.5$ a.u. corresponding to the mean value of the orbital radius for the $1s$ bound state.

Figure 2 shows the absolute value of ψ_f^I for two directions of $\mathbf{r}_P$, namely, $|\psi_f^I(+r_0\hat{\mathbf{v}},t)|$ and $|\psi_f^I(-r_0\hat{\mathbf{v}},t)|$. To have a reference as $t\rightarrow+\infty$ we also display $|\psi_f^{\mathrm{CDW}}|$, which tends to the proper limit as t increases. By defining the arguments of the wave functions, θ_f^I and θ_f^{CDW}, as $\psi_f^I = |\psi_f^I|\exp(i\theta_f^I)$ and $\psi_f^{\mathrm{CDW}} = |\psi_f^{\mathrm{CDW}}|\exp(i\theta_f^{\mathrm{CDW}})$, respectively, we find that θ_f^I and θ_f^{CDW} are quite like each other. From Fig. 2 it becomes evident that ψ_f^I does not satisfy the CBC, i.e., ψ_f^I does not tend to ϕ_f^∞ as $t\rightarrow+\infty$. We also observe that for the case $\mathbf{r}_P = r_0\hat{\mathbf{b}}$ (not shown here) the discrepancy between ψ_f^I and ψ_f^{CDW}, in the t range considered in Fig. 2, is in the order of the numerical uncertainty. Therefore, the departure of ψ_f^I from the proper limit is more important for $\mathbf{r}_P$ in the direction of $\mathbf{v}$ than in the perpendicular direction.

A crude estimation of ψ_f^I for large t can be derived from Eq. (1) by taking *first* the limit as $t\rightarrow+\infty$ and making *afterwards* a perturbative expansion. In first order the asymptotic deviation, defined as $\Delta_f^I(\mathbf{r}_P,t) = \psi_f^I(\mathbf{r}_P,t) - \phi_f^\infty(\mathbf{r}_P,t)$ as $t\rightarrow+\infty$, reads

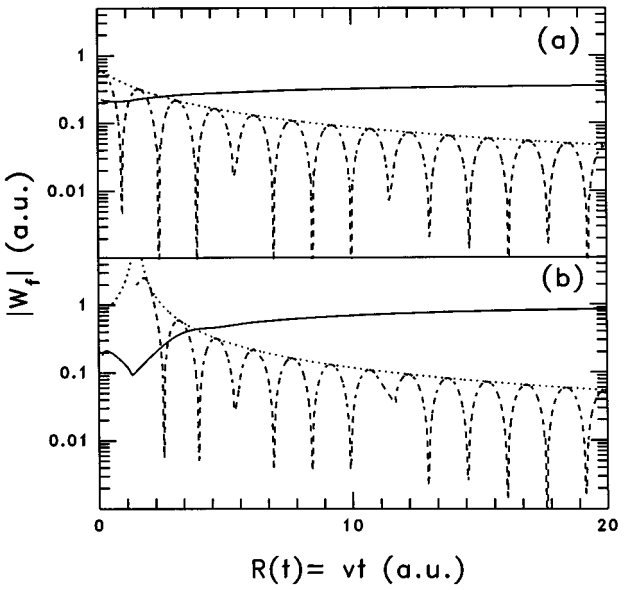

FIG. 3. Similar to Fig. 2 for the module of the perturbative potential W_f. Dotted line, absolute value of the Coulomb potential $-Z_T/r_T$.

$$\Delta_f^I(\mathbf{r}_P,t) \simeq -\frac{Z_T}{v^2}\phi_f^\infty(\mathbf{r}_P,t)[\ln\alpha(t)-1] \times \hat{\mathbf{v}}\cdot\nabla_{\mathbf{r}_P}\ln[\varphi_f(\mathbf{r}_P)] + \mathcal{O}\left(\frac{Z_T}{v^3}\right). \tag{6}$$

From this expression two points can be qualitatively observed in accordance with the exact numerical calculation. First, for ns final electronic states $\Delta_f^I(\mathbf{r}_P,t)\propto\hat{\mathbf{v}}\cdot\hat{\mathbf{r}}_P$, and this dependence clearly describes the asymptotic behavior of ψ_f^I for different directions of $\mathbf{r}_P$, as observed in Fig. 2. And second, $\Delta_f^I(\mathbf{r}_P,t)$ vanishes as the velocity increases.

For high velocities it is found that ψ_f^I and ψ_f^{CDW} show a good agreement in almost the whole relevant range of t values, the discrepancy being only a few percent. Further, as the velocity tends to infinity the impulse approximation, which uses ψ^I in one channel and the nonperturbed wave function in the other one, converges to the second order Born approximation, while the CDW approximation that employs ψ^{CDW} in both channels does not [10].

In the impact parameter treatment the perturbative potential W_f^I associated to ψ_f^I reads

$$W_f^I(\mathbf{r}_P,t) = \frac{1}{\psi_f^I}(\mathbf{r}_P,t)\left(H - i\frac{d}{dt}\right)\psi_f^I(\mathbf{r}_P,t) = \frac{f_e(\mathbf{r}_P,t)}{\psi_f^I(\mathbf{r}_P,t)}\int\frac{d\mathbf{k}}{(2\pi)^{3/2}}\left(\frac{k^2}{2}-\frac{Z_P}{r_P}-\varepsilon_f\right) \times\widetilde{\varphi_f}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}_P)D^-(Z_T,\mathbf{v}+\mathbf{k};\mathbf{r}_T), \tag{7}$$

where H is the electronic Hamiltonian and Z_P is the projectile charge. Note that the peaking approximation that leads from ψ_f^I to ψ_f^{CDW} does not conduct from W_f^I to the perturba-

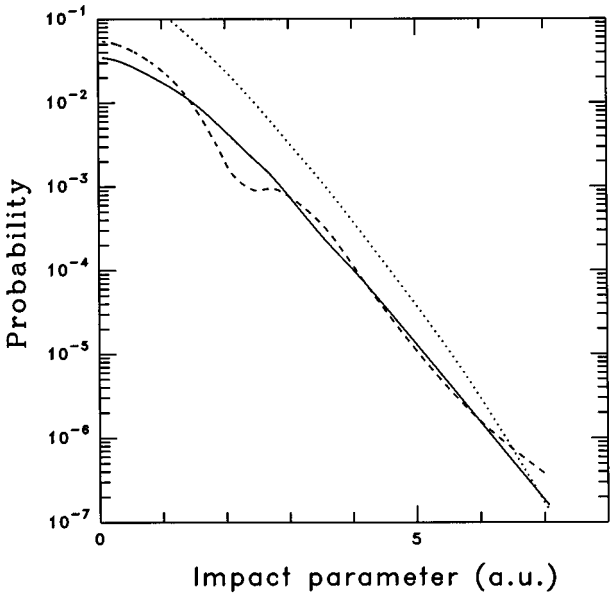

FIG. 4. Transition probability for the process $H^+ + H(1s) \rightarrow H(1s) + H^+$ at $v = 2$ a.u., as a function of the impact parameter b (in atomic units). Theories: solid line, EI approximation; dashed line, CDW approximation; dotted line, Brinkman-Kramers approximation.

tive potential corresponding to ψ_f^{CDW} (W_f^{CDW}), as was argued by Dewangan and Eichler [8] to perceive the ill-behavior of ψ_f^I.

In Fig. 3 we plot $|W_f^I|$ along with $|W_f^{\mathrm{CDW}}|$ and the absolute value of the Coulomb potential $V_T = -Z_T/r_T$. Again we consider two directions of $\mathbf{r}_P$, namely, $\mathbf{r}_P = +r_0\hat{\mathbf{v}}$ and $\mathbf{r}_P = -r_0\hat{\mathbf{v}}$. From Fig. 3 it can be seen that in both cases $|W_f^I|$ increases as $R(t) = vt$ grows. This inconsistency with the scattering theory is certainly a direct consequence of the improper limit of ψ_f^I. Anyway, it should be observed that in average $|W_f^I| < |W_f^{\mathrm{CDW}}|$ for $R(t) < 2$ a.u., i.e., at short times [in the proximities of $R(t) = vt \sim 0$] where the most important contribution to the transition amplitude takes place.

For the case $\mathbf{r}_P = -r_0\hat{\mathbf{v}}$ [Fig. 3(b)] the potential W_f^{CDW} is not well defined for $R(t) < r_0$, this behavior being consistent with the fact that W_f^{CDW} is not well behaved for negative time. This problem was pointed out by Crothers [11], who devised a symmetrized version of the CDW approximation to solve it. From Fig. 3(b) we can also observe that at $R(t) \simeq r_0$ ($\mathbf{r}_P \simeq 0$), $|W_f^I|$ is much smaller than $|W_f^{\mathrm{CDW}}|$. Again, we found that the separation between $|W_f^I|$ and $|W_f^{\mathrm{CDW}}|$ is more important for $\mathbf{r}_P$ in the direction of $\mathbf{v}$ than in the perpendicular direction. For $\mathbf{r}_P$ perpendicular to $\mathbf{v}$ the separation is of the order of the numerical uncertainties.

Finally, we attempt to explain why the use of ψ_f^I permits us to describe a large variety of collisional data, even thought this wave function does not satisfy the CBC, as observed before. Two reasons are posed.

First, the most important contribution to the transition amplitude comes from the region of small values of t, where ψ_f^I and W_f^I behave rather soundly. For example, in the collision system considered in this work the capture probability reaches 90% of its final value at $R(t) = vt \sim 3$ a.u.; hence the transition amplitude is mostly defined in the region corresponding to small values of $R(t)$.

Second, when ψ_f^I is averaged by integrating on all possible directions of $\mathbf{r}_P$, i.e., $\langle \psi_f^I \rangle = \int d\hat{\mathbf{r}}_P \psi_f^I(\mathbf{r}_P, t)$, this value differs from that corresponding to ψ_f^{CDW} in much less than 10% in the range $3 \text{ a.u.} \leqslant R(t) \leqslant 30$ a.u. Therefore, the values of ψ_f^I for different directions of $\mathbf{r}_P$ should partially cancel their wrong contributions for large $R(t)$ as they are integrated to obtain the transition amplitude.

As a further examination it is useful to inspect the transition probability as a function of the impact parameter b, as shown in Fig. 4. We observe that EI and CDW approximations give very similar probabilities in the range $3 \text{ a.u.} \leqslant b \leqslant 6$ a.u., and both methods largely differ from the first order Brinkman-Kramers results. At $b = 6$ a.u. the transition probability is four orders of magnitude smaller than the maximum value at $b = 0$, and consequently the discrepancy—if any—between EI and CDW transition probabilities for $b > 6$ a.u. is unimportant for evaluating the total cross section. Since large impact parameters correspond necessarily to large internuclear distances, the agreement between EI and CDW approximations for $3 \text{ a.u.} \leqslant b \leqslant 6$ a.u. would indicate that the improper limit of ψ_f^I may be unessential, at least for the calculation of total cross sections.

In conclusion, by inspecting the numerical results we have shown that ψ_f^I does not satisfy the CBC, as observed by Belkić *et al.* [7] and Dewangan and Eichler [8], and in contrast with our previous assertion [6]. However, arguments have been put forward to explain the success of ψ_f^I in describing a large variety of capture results, including symmetric collisional systems at intermediate impact velocities. These arguments suggest that the asymptotic failure has a minor influence at level to the total cross section. We think that the ill-asymptotic condition of the impulse wave function may be counterbalanced by a sound description of the collisional process at small distances as well as the proper normalization.

[1] J. P. Coleman and M. R. C. McDowell, Proc. Phys. Soc. **85**, 1097 (1965); J. P. Coleman and S. Trelease, J. Phys. B **1**, 172 (1968); J. P. Coleman, *ibid*. **1**, 567 (1968).

[2] J. P. Coleman, *Case Studies in Atomic Physics* (North-Holland, Amsterdam, 1969), Vol. 1, p. 100.

[3] J. S. Briggs, J. Phys. B **10**, 3075 (1977).

[4] D. H. Jakubaβa-Amundsen and P. A. Amundsen, Z. Phys. A **297**, 203 (1980).

[5] M. R. C. McDowell and J. P. Coleman, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam, 1970), pp. 354 and 408.

[6] M. S. Gravielle and J. E. Miraglia, Phys. Rev. A **44**, 7299

(1991); **51**, 2131 (1995); **52**, 851 (1995).
[7] Dz. Belkić, R. Gayet, and A. Salin, Phys. Rep. **56**, 279 (1979).
[8] D. P. Dewangan and J. Eichler, Phys. Rep. **247**, 59 (1994).
[9] The momentum-space wave function $\widetilde{\varphi}_l(\mathbf{k})$ has a sharp maximum at $\mathbf{k}=\mathbf{0}$ for the s-bound states. For other low l states the maximum of $\widetilde{\varphi}_l(\mathbf{k})$ is found to be displaced, depending on the magnetic quantum number m.
[10] R.D. Rivarola and J. E. Miraglia, J. Phys. B **15**, 2221 (1982).
[11] D. S. F. Crothers, J. Phys. B **15**, 2061 (1982); D. S. F. Crothers and L. J. Dubé, Adv. Atom. Mol. **30**, 287 (1993).