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Off-shell distortions of multichannel atomic processes

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Any multichannel problem can be reduced to a succession of two-body events. However, these basic building blocks of many-body theories do not correspond to elastic processes but are off-the-energy-shell. In view of this difficulty, the great majority of the Distorted-Wave models includes a subsidiary approximation where these off-shell terms are arbitrarily forced to lie on the energy shell. At a first glance, since the energy deficiency is negligible for high enough velocities, the on-shell assumption seems to be completely justified. However, for the case of Coulomb interactions, the two-body off-shell distortions have branch-point singularities on the on-shell limit. In this article we demonstrate that these singularities might produce sizeable distortions of multiple scattering amplitudes, mainly when dealing with ion-ion collisions. Finally, we propose a method of including these distortions that might lead to better results that removing them completely.

1. Introduction

A non-relativistic many-body theory was first formulated in the 1950s by Kenneth M. Watson [1]. In the following decade Ludvig Dmitrievich Faddeev [2–4] introduced a celebrated three-body symmetric version of Watson's theory, and provided a clear and mathematically complete analysis of its convergence. Through these theories, any multichannel collision can be iteratively reduced to two-body scattering processes. The catch, however, is that these two-body collisions are off-the-energy-shell. This means that in each of them, the initial, intermediate and final energies are not necessarily equal to each other, as they should be if the process were elastic.

This leads to some serious difficulties when Coulomb interactions are involved. It is fair to say that these difficulties do not arise from their calculation, since mathematically well defined representations of off-shell two-body Coulomb wave functions and transition matrix elements are known [5], but from an anomalous on-the-energy-shell limiting behavior, namely a branch-point singularity, that is characteristic of any long-range interaction. The energy deficiency is negligible for high enough velocities [6], but the presence of this branch-point leaves this on-shell limit undefined, and therefore replacing the off-shell Coulomb wave function by its on-shell version is not valid.

Already in the early 1970s it was known that these singularities produce the leading contributions to multiple-scattering amplitudes in rearrangement and scattering collisions at high energies [7–9]. However, in following years, this problem failed to be dully analyzed and in the end became discarded and even ignored. For instance, the very same definition of the initial and final states in Continuum Distorted Wave (CDW) theories (see, e.g., [10] and citing articles), where the two-body distortions are incorporated as multiplicative factor (i.e. Confluent Hypergeometric Functions) instead of convolutions of their off-shell counterparts over some intermediate momenta, is an unmistakable fingerprint of this on-shell assumption.

One of the few theoretical studies where this problem was taken into account was the Channel–Distorted Strong-Potential Born (DSPB) approximation for highly asymmetric mechanical and radiative ion-atom charge-exchange processes [11–16]. In these models, the on-shell singularities of the intermediate states were shown to produce a sizeable effect, even though the separation from the energy shell was small. Against this argument, it was argued that the Coulomb singularities are nonphysical, since the interactions are always screened at large enough distances [17,18]. However, even for moderate screening ranges, the difference between the off-shell and on-shell approximations is known to produce very strong distortions of multiple-scattering amplitudes [11,16]. In most cases, approximating these distortions by

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means of actual Coulomb singularities was shown to produce much better results that removing them completely.

In this paper, we present a general framework for the description of off-shell effects in Atomic Collisions. Even though we restrict ourselves to consider three-body phenomena, the theory can be straightforwardly extended to more general few-body phenomena.

2. The on-shell approximation revisited

Let us consider a three-body system consisting of an electron and an ion of charge Z' and mass M' in a bound state ϕ with (negative) energy ϵ, and another ion of charge Z and mass M in the continuum with momentum $\mathbf{P}$ (i.e. velocity $\mathbf{v} = \mathbf{P}/\mu$) with respect to the center-of-mass of the bound state. Here $\mu = M(1+M')/M'M$ is a reduced mass of the three-body system (atomic units are used throughout this article). For pedagogical and briefness reasons we will not study the ionization channel (i.e. with the three particles in the continuum). Coming back to the system under consideration, its exact outgoing (+) or ingoing (−) stationary scattering states read (see, e.g. [19]),

$$|\phi,\mathbf{P}\pm\rangle = \left[1 + G\left(\epsilon + \frac{P^2}{2\mu} \pm i\gamma\right)(V_o - V')\right]|\phi,\mathbf{P}\rangle, \quad (1)$$

where $|\phi,\mathbf{P}\rangle$ represents the system when the ion and the atom are infinitely separated in space representation. The full Green operator reads $G(z) = (z - H_o - V_o)^{-1}$, where H_o is the total kinetic energy operator, $V_o = V(r) + V'(r') + ZZ'/|\mathbf{r}-\mathbf{r}'|$ is the total potential energy between the three particles; and $V(r) = -Z/r$ and $V'(r') = -Z'/r'$ are the Coulomb interactions between the electron and the ions, while γ is a positive infinitesimal. Now, without any loss of generality, let us write,

$$|\phi,\mathbf{P}\pm\rangle = \int d\mathbf{p}\left[1 + G\left(\epsilon + \frac{P^2}{2\mu} \pm i\gamma\right)(V_o - V')\right]|\mathbf{p},\mathbf{P}\rangle\tilde{\phi}(\mathbf{p}). \quad (2)$$

where $\tilde{\phi}(\mathbf{p}) = \langle\mathbf{p}|\phi\rangle$ is the Fourier transform of the bound state ϕ. It is clear that the intermediate state

$$|\mathbf{p},\mathbf{P}\pm\rangle_{\delta\varepsilon} = \left[1 + G\left(\epsilon + \frac{P^2}{2\mu} \pm i\gamma\right)(V_o - V')\right]|\mathbf{p},\mathbf{P}\rangle \quad (3)$$

is off the energy shell by an amount $\delta\varepsilon = p^2/2 - \epsilon$. As it was previously explained, it is a standard practice in the vast majority of the perturbative models to assume that this "energy deficiency" $\delta\varepsilon$ is very small, and therefore to approximate the previous intermediate state by its on-shell version

$$|\mathbf{p},\mathbf{P}\pm\rangle = \left[1 + G\left(\frac{p^2}{2} + \frac{P^2}{2\mu} \pm i\gamma\right)(V_o - V')\right]|\mathbf{p},\mathbf{P}\rangle. \quad (4)$$

In particular, this represents the starting point for every Continuum Distorted Wave (CDW) theory [10]. Let us assume, for instance, the validity of Wick's argument [20], so as to disregard the ion-ion interaction, and consider the following CDW approximation

$$\langle\mathbf{r}',\mathbf{R}|\mathbf{p},\mathbf{P}\pm\rangle \approx D_\pm(\mathbf{r},\mathbf{k})\langle\mathbf{r}',\mathbf{R}|\mathbf{p},\mathbf{P}\rangle = \frac{1}{(2\pi)^3}D_\pm(\mathbf{r},\mathbf{k})\exp\left(i(\mathbf{p}\cdot\mathbf{r}' + \mathbf{P}\cdot\mathbf{R})\right), \quad (5)$$

where

$$D_\pm(\mathbf{r},\mathbf{k}) = e^{-\pi n/2}\Gamma(1 \pm in)_{1F_1}(\mp in, 1; \pm i(kr \mp \mathbf{k}\cdot\mathbf{r})), \quad (6)$$

is the distortion factor of the two-body Coulomb Continuum Stationary State in space representation for the interaction of the electron and the ion in the continuum, namely [21]

$$\langle\mathbf{r}|\mathbf{k}\pm\rangle = \frac{1}{(2\pi)^{3/2}}D_\pm(\mathbf{r},\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{r}). \quad (7)$$

Here $n = -Z/k$and ${}_1F_1(a,c;z)$ is the Confluent Hypergeometric Function [22].

This CDW approximation is intended to improve the description of the motion of an electron attached to an ion by incorporating a continuum distortion produced by another ion. Initially created for studying charge exchange collisions, CDW theories were subsequently generalized in different contexts and applied to ionization collisions and other reactions, and for a large variety of collision partners, ranging from electrons and positrons to highly charged ions. However, it is clear that, in all their different variations [23], CDW theories implicitly incorporate an on-shell approximation.

However, even though in most applications it might be sound to assume that the energy deficiency is small, this does not necessary implies that the on-shell limit 4 would be valid. The reason is that for Coulomb interactions, the on-shell limit is not well-defined. In fact, as it is explained in the following section, it present a branch-point singularity whose effect on the analysis of multichannel collision processes should not be ignored.

3. Two-body off-shell coulomb continuum states

Let us now consider the same two-body state $|\mathbf{k}\pm\rangle$ of the previous section, but allowing for a difference between the energy in the Green operator and that of the plane wave, namely

$$|\mathbf{k}\pm\rangle_{\delta\varepsilon} = \left(1 + (k^2/2 - \delta\varepsilon \pm i\gamma - H)^{-1}V\right)|\mathbf{k}\rangle, \quad (8)$$

with $H = -\nabla_{\mathbf{r}}^2/2 - Z/r$.

For most quantum-mechanical systems, this off-shell continuum state can not be evaluated in close form. However, mathematically well defined, even analytical expressions of this state and the corresponding T-matrix element are well known and have been extensively described in the literature (see, e.g. [8]). Here we are not interested in these analytical representations for arbitrary values of $\mathbf{k}$ and $\delta\varepsilon$, but only for their expressions in the vicinity of the on-shell limit $\delta\varepsilon \to 0$. Actually, in this limit, the incoming (−) and outgoing (+) off-shell scattering states can be approximated by [24]

$$|\mathbf{k}\pm\rangle_{\delta\varepsilon} \approx g^\pm(k,\delta\varepsilon)|\mathbf{k}\pm\rangle, \quad (9)$$

where

$$g^\pm(k,\delta\varepsilon) = \frac{\Gamma(1 \mp in)}{e^{\pi n/2}}\left(\frac{\delta\varepsilon \mp i\gamma}{2k^2 \pm i\gamma}\right)^{\pm in}. \quad (10)$$

This simple result implies that $g^\pm(k,\delta\varepsilon)$ does not approaches unity for $\delta\varepsilon \to 0$ but reaches different values on each side of the branch-point at the on-shell limit, namely

$$g^\pm(k,\delta\varepsilon) \approx e^{-\pi n/2}\Gamma(1 \mp in)\left|\frac{\delta\varepsilon}{2k^2}\right|^{\pm in} \quad (11)$$

for $\delta\varepsilon > 0$ and

$$g^\pm(k,\delta\varepsilon) \approx e^{\pi n/2}\Gamma(1 \mp in)\left|\frac{\delta\varepsilon}{2k^2}\right|^{\pm in} \quad (12)$$

for $\delta\varepsilon < 0$. Thus, even though in most applications it might be sound to assume that the energy deficiency is small, the effect of the branch-point singularities is not necessarily so, and therefore has to be taken into account, something that CDW approximations, by only incorporating a Coulomb distortion factor $D_{\pm}(\mathbf{r},\mathbf{k})$, do not. Instead, we are proposing a method to correct on-shell perturbative approximations, by multiplying any distortion factor $D_{\pm}(\mathbf{r},\ \mathbf{k})$ by a term $g^{\pm}(k,\delta\varepsilon)$, namely,

- Replace $D_{\pm}(\mathbf{r},\mathbf{k})$ by $g^{\pm}(k,\delta\varepsilon)\times D_{\pm}(\mathbf{r},\mathbf{k})$,

in order to take into account the corresponding branch-point singularity. This is the main result of the present article.

Now, in order to quantify this off-shell distortion, study its relevance and analyze whether and under which conditions it can be disregarded or has be taken into account, in the following section we make some sensible approximations so as to obtain a simple estimation of its magnitude.

4. Off-shell distortion factor

Let us apply the previous theory to a general transition matrix element either in post or prior forms,

$$T^{+}=\langle\Psi_f|V_f|\phi,\mathbf{P}+\rangle \tag{13}$$

and

$$T^{-}=\langle\phi,\mathbf{P}-|V_i|\Psi_i\rangle. \tag{14}$$

Here $|\Psi_f\rangle$ ($|\Psi_i\rangle$) and V_f (V_i) are the asymptotic state and potential of the final (initial) channel [19]. Now, let us assume that we apply a CDW correction on the state $|\phi,\mathbf{P}\pm\rangle$. In this case, as explained in the previous section and due to the implicit on-shell approximation, we should incorporate the corresponding $g^{\pm}$ factors, namely

$$T^{+}\approx\int \mathrm{d}\mathbf{p}g^{+}(k,\delta\varepsilon)\langle\Psi_f|V_f|\mathbf{p},\mathbf{P}+\rangle\tilde{\phi}(\mathbf{p}) \tag{15}$$

or

$$T^{-}\approx\int \mathrm{d}\mathbf{p}g^{-}(k,\varepsilon)\tilde{\phi}^{*}(\mathbf{p})\langle\mathbf{p},\mathbf{P}-|V_i|\Psi_i\rangle, \tag{16}$$

Now, by applying a full peaking approximation [16], where $\mathbf{p}$ is ignored compared to the projectile velocity $\mathbf{v}$, we obtain

$$T^{\pm}\approx M_{\pm}\times T^{\pm}_{IA}, \tag{17}$$

where

$$T^{+}_{IA}=\langle\Psi_f|V_f|0,\mathbf{P}+\rangle\int \mathrm{d}\mathbf{p}\tilde{\phi}(\mathbf{p}) \tag{18}$$

and

$$T^{-}_{IA}=\langle 0,\mathbf{P}-|V_i|\Psi_i\rangle\int \mathrm{d}\mathbf{p}\tilde{\phi}^{*}(\mathbf{p}), \tag{19}$$

are the so called Impulse Approximations (IA), which are valid at sufficiently high velocities [16]. On the other hand, the distortion factors

$$M_{+}=M^{*}_{-}=\int \mathrm{d}\mathbf{p}g^{+}(k,\delta\varepsilon)\tilde{\phi}(\mathbf{p})\Big/\int \mathrm{d}\mathbf{p}\tilde{\phi}(\mathbf{p}), \tag{20}$$

incorporate the effect of the off-shell distortion on the electron–ion continuum.

For a 1s state, and assuming that v is large enough so that $|\epsilon|\ll v^2/2$, a straightforward calculation shows that

$$M_{\pm}=\frac{1}{\sqrt{\pi}}\left(\frac{|\epsilon|}{2v^2}\right)^{\pm i\nu}\frac{\Gamma(1/2\mp i\nu)}{e^{\pi\nu/2}(1\mp i\nu)}, \tag{21}$$

where we have defined $\nu=-Z/v$. Its squared modulus reads,

$$|M_{\pm}|^2=\frac{2}{(1+\nu^2)(1+e^{2\pi\nu})}. \tag{22}$$

We see in Fig. 1 that this off-shell distortion factor goes to zero for small energies (i.e. large values of ν) and tends to 1 for large energies (i.e. small values of ν). It reaches its maximum value, $|M|^2\approx 1.60387$ for $\nu\approx -0.35$.

The $|\epsilon|\ll v^2/2$ condition establishes an upper limit to the range of values of ν for which Eqs. 21 and 22 are valid. However, we clearly see in Fig. 1 that even in the most astringent cases, large departures from the on-shell limit $|M|^2=1$ can be reached for very small values of $|\nu|$. Let us consider, for instance, the following linear approximation,

$$|M|^2\approx 1-\pi\nu. \tag{23}$$

We see, for instance, that a departure of more than 20% from the on-shell limit can be reaches by velocities as large as $v\approx 15Z$ (i.e. $|\nu|\approx 0.067$), well into the perturbative regime. Even the value at the maximum corresponds to a velocity $v\approx 2.86Z$.

5. Conclusions

The simple results obtained in the previous section demonstrate that standard Impulsive and Continuum Distorted Wave models, by approximating the intermediate Coulomb states by their on-shell versions, might be incorporating a sizable systematic error in the evaluation of multichannel cross sections which should be pondered and eventually corrected by means of the simple proposal stated at the end of Section 3.

In order to further exemplify this assertion, in Fig. 2 we show the off-shell distortion factor $|M|^2$ for a system consisting of a nude Carbon ion of relative velocity v (i.e. energy $E=v^2/2$) with respect to a Hydrogen atom in its ground state. It is clearly seen that the magnitude of the off-shell distortion might be over 40 % for intermediate and large energies.

Let us finally note that in some variations of the continuum distorted wave model, the Coulomb distortion might be applied onto a couple of intermediate two-body systems. In the framework of the procedure proposed in the present article, each of both Coulomb distortion D should have to be corrected by the corresponding off-shell factor g in order to take into account the branch-point singularities at the on-shell limits. In this case, the calculation of the distortion factor M follows, *mutatis mutandis*, the same procedure implemented in the present article. In particular, it can be

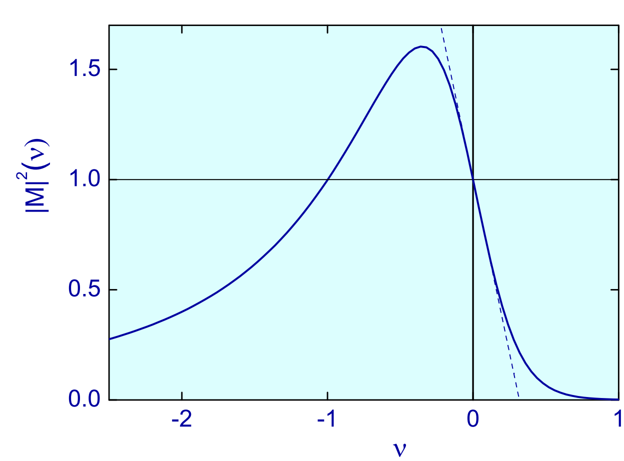

Fig. 1. Off-shell distortion factor $|M(\nu)|^2$ and its linear approximation (dashed line), as a function of the dimensionless parameter $\nu=-Z/v$. The case of negative ions (i.e. $\nu>0$) has also been included.

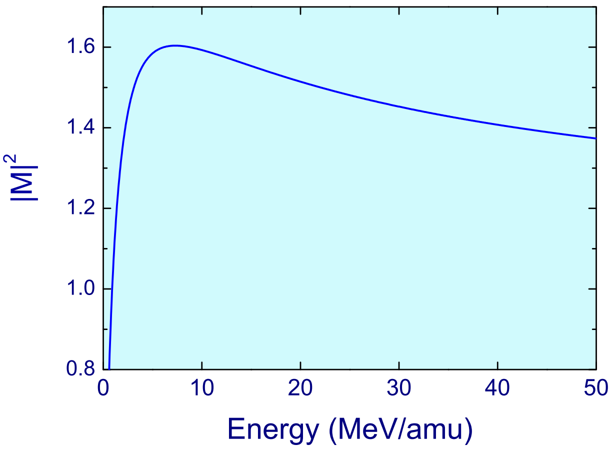

Fig. 2. Off-shell distortion factor $|M|^2$ for a C_{6+} + H (1s) system as a function of the relative energy *E*.

demonstrated that if one of the two parameters *ν* corresponding to each of the two Coulomb continuum distortions is equal to zero, we recover the expression for a single distortion, as described in Section 3.

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