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Semiclassical Coulomb interaction

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The semiclassical Coulomb excitation interaction is at times expressed in the Lorentz gauge in terms of the electromagnetic fields and a contribution from the scalar electric potential. We point out that the potential term can make spurious contributions to excitation cross sections, especially when the decay of excited states is taken into account. We show that, through an appropriate gauge transformation, the excitation interaction can be expressed in terms of the electromagnetic fields alone.

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Coulomb excitation has proven itself as an important tool for studying the structure of both stable and exotic nuclei [1–4]. The phenomenon has been well-studied in a nonrelativistic context [5] and studied perturbatively in a relativistic one [6] by Alder and Winther. More recent experimental studies have shown the need to consider multiple Coulomb excitation at relativistic energies [2–4] and, although the formalism of Ref. [6] can be extended to permit such calculations, it is not easy to implement [7,8]. An alternative semiclassical form of the Coulomb excitation interaction was presented in Ref. [9] and refined in a more recent analysis [10]. There, the Coulomb excitation interaction is expressed in the Lorentz gauge in terms of the electromagnetic fields and the scalar electric potential. This mixed representation of the interaction yields the results of Winther and Alder when used perturbatively and is adequate for describing single and multiple excitation of states of zero width at incident energies lower than about 2 GeV/nucleon, where the results are almost identical to those obtained by directly using the electromagnetic fields, as in a classical treatment of the problem. At higher energies, coupled channel calculations in the mixed and field representations yield results that are increasingly discrepant, as the excitation cross section of the mixed representation quickly grows to absurdly large values. Similar discrepancies have also been observed in a recent comparison of relativistic Coulomb excitation in the Lorentz and Coulomb gauges [11].

Electromagnetic processes, such as Coulomb excitation, should be gauge-invariant. Truncation of the coupled-channels model space can spoil this invariance however [12], permitting spurious, but gauge-removable terms, such as the potential term in the Lorentz interaction, to contribute to the cross sections. Baltz, Rhoades-Brown, and Weneser have seen similar large effects in their extensive study of e^+e^- production [13–15] and have found as well that, when performed with care, an appropriate gauge transformation can greatly simplify calculations.

In the case of the mixed interaction of the Lorentz gauge, the effects of the spurious potential term are exacerbated even further when the excited states are allowed to decay. The mixed representation then yields large, unphysical cross sections at all incident energies, due to the loss of flux after excitation by the long-range potential term. The production cross section of the decay products of a dipole transition, in particular, grows as the square of the Lorentz factor γ. This makes a treatment of multiple Coulomb excitation incorporating fluctuation contributions, such as those of the Brink-Axel type [16–19], unviable in the mixed representation, since finite widths are a fundamental component of such models.

Following, we first provide an estimate of the production cross section of the decay products of a dipole transition induced by the long-range potential term. We then demonstrate, through an appropriate gauge transformation, that the Coulomb excitation component of the interaction can indeed be expressed in terms of the electromagnetic fields alone. Aside from making a satisfying parallel with the classical case, the pure field representation of the excitation interaction, known as the multipolar or Poincaré gauge [20], provides physically reasonable cross sections even when the excited states decay [18]. A similar expression has been used in the treatment of Coulomb excitation of plasmon resonances in metallic clusters [21].

In the usual semiclassical approximation to heavy-ion scattering, the relative motion is described by a classical trajectory. The projectile-target interaction is then a time-dependent function determined by this trajectory. The semiclassical form of the electromagnetic interaction Hamiltonian is given by

$$V(t) = \int d^3x \left(\rho(\vec{x},t)\varphi(\vec{x},t) - \frac{1}{c}\vec{J}(\vec{x},t)\cdot\vec{A}(\vec{x},t) \right), \quad (1)$$

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where $\varphi(\vec{x}, t)$ and $\vec{A}(\vec{x}, t)$ are the scalar and vector electromagnetic potentials due to the projectile, for which

$$\vec{E}(\vec{x}, t) = -\nabla\varphi(\vec{x}, t) - \frac{1}{c}\frac{\partial \vec{A}(\vec{x}, t)}{\partial t}$$

and

$$\vec{B}(\vec{x}, t) = \nabla \times \vec{A}(\vec{x}, t), \tag{2}$$

and $\rho(\vec{x}, t)$ and $\vec{J}(\vec{x}, t)$ are the charge and current density operators of the target nucleus. In high-energy collisions, one usually uses the Liénard-Wiechert potential, which is the retarded electromagnetic potential, in the Lorentz gauge, of a charged particle moving on a straight line trajectory.

In Ref. [9] the Liénard-Wiechert potential was used to obtain the Coulomb interaction for multipole excitation of a target nucleus in a mixed representation that depends on both the electric field and the scalar electric potential. The interaction inducing transverse dipole excitations is written in terms of the electric field alone. Due to the contribution of the vector potential, the interaction inducing longitudinal transitions also includes a potential-like term. It can be written as

$$V_{1\parallel}(b, t) = V_0 \left[\frac{\gamma v t}{(b^2 + (\gamma v t)^2)^{3/2}} - e^{-i\omega t}\frac{\beta\gamma}{c}\frac{d}{dt}\left(\frac{e^{i\omega t}}{(b^2 + (\gamma v t)^2)^{1/2}}\right)\right], \tag{3}$$

with b being the impact parameter, v the projectile velocity, $\hbar\omega$ the excitation energy, $\beta = v/c$, and γ the associated Lorentz factor. The quantity V_0 represents the product of the projectile charge, the matrix element for dipole excitation and numerical factors. (Note that the factor $\mathcal{E}_2(\tau)$ defined in Eq. (26) of Ref. [9] must be divided by τ^2 to provide the correct expression, which can be found in Ref. [22].)

Let us now consider the time evolution of three states: the ground state, the longitudinal dipole mode excited by Coulomb excitation, and the residual state fed by the decay of the latter. The time evolution equations of the ground-state and dipole-mode amplitudes, $a_0(b, t)$ and $a_{1\parallel}(b, t)$, respectively, can be written in the interaction picture as [18]

$$\begin{aligned} i\hbar\frac{d}{dt}a_0(b, t) &= V_{1\parallel}(b, t)e^{-i\omega t}a_{1\parallel}(b, t), \\ i\hbar\frac{d}{dt}a_{1\parallel}(b, t) &= V_{1\parallel}(b, t)e^{i\omega t}a_0(b, t) - i\frac{\Gamma}{2}a_{1\parallel}(b, t), \end{aligned} \tag{4}$$

where Γ is the width of the dipole resonance. The residual state is fed incoherently by the decay of the dipole mode. The time evolution equation for its occupation probability can be written as

$$\frac{dP_{\rm dec}}{dt}(b, t) = \frac{\Gamma}{\hbar}|a_{1\parallel}(b, t)|^2. \tag{5}$$

Coupled coherent-incoherent evolution equations such as these can be consistently formulated in terms of the density matrix, as shown in Refs. [18,19]. The formulation above is sufficient for our purposes here.

Since the interaction tends to zero as $b \to \infty$, first order perturbation theory is valid at large values of the impact parameter, where depletion of the ground-state and occupation of the longitudinal excitation can be neglected on the right side of the equation. We can then approximate the amplitude for excitation of the longitudinal mode by retaining only the second term in $V_{1\parallel}(b, t)$, which decreases as b^{-1}, as

$$\begin{aligned} a_{1\parallel}(b, t) &\approx -\frac{i}{\hbar}\int_{-\infty}^{t} ds\, V_{1\parallel}(b, s)e^{i\omega s} \\ &= iV_0\frac{\beta\gamma}{\hbar c}\frac{e^{i\omega t}}{(b^2 + (\gamma v t)^2)^{1/2}} + \mathcal{O}\left(\frac{1}{b^3}\right). \end{aligned} \tag{6}$$

It is clear that the contribution of the $1/b$ term vanishes as $t \to \infty$ and that it thus makes no net contribution to the excitation, when no flux is absorbed from the excited mode and ground-state depletion is negligible. These are the assumptions used in the usual perturbative calculation of the asymptotic amplitude. When the dipole mode decays, however, this term does contribute to the occupation of the residual state, with the asymptotic occupation probability of that state being

$$\begin{aligned} P_{\rm dec}(b) &= \frac{\Gamma}{\hbar}\int_{-\infty}^{\infty} dt|a_{1\parallel}(b, t)|^2 \\ &\approx \frac{\beta\gamma}{b}\frac{\Gamma V_0^2}{(\hbar c)^3}. \end{aligned} \tag{7}$$

Using this perturbative probability, we can estimate the cross section for production of the decay product to be at least

$$\sigma_{\rm dec} \approx 2\pi\int_{b_{\rm min}}^{b_{\rm max}} P_{\rm dec}(b)bdb = 2\pi\beta\gamma\frac{\Gamma V_0^2}{(\hbar c)^3}(b_{\rm max} - b_{\rm min}), \tag{8}$$

where $b_{\rm min}$ is the minimum value of the impact parameter at which the perturbative approximation is valid and $b_{\rm max} = \gamma v/\omega_0$ is determined by limiting the impact parameter to values for which the adiabaticity parameter $\xi = \frac{\omega_0 b}{\gamma v}$ is less than one [6], with $\hbar\omega_0$ the minimum value of the excitation energy considered as contributing to the dipole mode. The resulting cross section thus grows with energy as γ^2.

The absurd result furnished by the above estimate is confirmed by the full coupled-channels calculations given in Table I. The calculations were performed for the system ^{208}Pb + ^{208}Pb using the three channels described above, with a dipole excitation energy of $\hbar\omega = 13.4$ MeV, a reduced matrix element in accord with the giant dipole resonance sum rule and a minimum excitation energy of $\hbar\omega_0 = 8$ MeV. We have labeled the cross sections of the table as dipole-mode excitation cross sections. In the case of zero-width, they are in fact the cross sections for excitation of this mode. In the case of finite

TABLE I. Dipole mode excitation cross section of ^{208}Pb incident on ^{208}Pb using the pure field and the mixed (Lorentz) representations of the interaction.

Representation	Γ(MeV)	σ(b) at 1 GeV/nucleon	σ(b) at 10 GeV/nucleon
Field	0	4.26	13.98
Field	4	4.53	13.73
Mixed	0	4.46	98.84
Mixed	4	15.09	334.06

width, the values represent the flux that was excited to the dipole mode to later decay to the residual state.

Similar calculations were reported in Ref. [22]. Comparison of their zero-width results with ours and with those of Ref. [24] leads us to conclude that they performed the calculations with the pure field form that we are advocating. The trend of their finite-width results also leads us to infer that they took the width into account in the decay of the dipole mode but not in its excitation.

We thus conclude that the spurious potential term in the interaction produces absurdly large cross sections when decay of the excited state is taken into account. Even when the width of the state is zero, this term, abetted by depletion of the ground-state, introduces contributions that increase with incident energy and also lead to absurdly large cross sections, such as those at 10 GeV/nucleon shown in the last column of the table. The unphysical results in both cases are attributable to the unphysical $1/b$ term in the truncated coupled-channels calculations. We can also argue against such a term on simple physical grounds: we expect the polarization that produces the excitation of the target nucleus to depend on the gradient of the potential, that is the electric field, rather than the potential itself. In the following, we will show how the electromagnetic interaction Hamiltonian can be recast in a more physical form.

We want to obtain the first few terms contributing to the interaction in the expansion of the electromagnetic fields about the center of the target nucleus, $\vec{x} = 0$. Such an expansion is reasonable if the fields are slowly varying over the extent of the nucleus.

We thus take

$$\int d^3x\, \rho(\vec{x},t)\varphi(\vec{x},t) \approx \int d^3x\, \rho(\vec{x},t) \times \left(\varphi_0(t) + \vec{x}\cdot\nabla\varphi_0(t) + \frac{1}{2}\vec{x}\vec{x}\cdot\nabla\nabla\varphi_0(t) + \cdots\right) \quad (9)$$

and

$$\int d^3x\, \vec{J}(\vec{x},t)\cdot\vec{A}(\vec{x},t) \approx \int d^3x\, \vec{J}(\vec{x},t) \cdot(\vec{A}_0(t) + \vec{x}\cdot\nabla\vec{A}_0(t) + \cdots), \quad (10)$$

where the subscript 0 on the fields and their derivatives denotes the evaluation of these quantities at the point $\vec{x} = 0$.

Evaluation of the scalar potential terms is straightforward. Evaluation of the vector potential terms requires a bit more work. We use the continuity equation,

$$\nabla\cdot\vec{J} + \frac{\partial\rho}{\partial t} = 0, \quad (11)$$

to obtain two supplementary identities [23]:

$$\int d^3x\, J_k = \int d^3x\, [\nabla\cdot(x_k\vec{J}) - x_k\nabla\cdot\vec{J}] = \int d^3x\, x_k\frac{\partial\rho}{\partial t}, \quad (12)$$

where the integral of the exact divergence is zero due to the finite extent of $\vec{J}$, and, after a similar calculation,

$$\int d^3x\, (J_k x_i + J_i x_k) = \int d^3x\, x_k x_i \frac{\partial\rho}{\partial t}. \quad (13)$$

Using the first of these, we can write

$$\int d^3x\, \vec{J}(\vec{x},t)\cdot\vec{A}_0(t) = \sum_k \int d^3x\, J_k(\vec{x},t)A_{0k}(t) = \sum_k \int d^3x\, \frac{\partial\rho}{\partial t}x_k A_{0k}(t) = \int d^3x\, \frac{\partial\rho}{\partial t}\vec{x}\cdot\vec{A}_0(t). \quad (14)$$

Using the second, we find, with a bit more work,

$$\int d^3x\, \vec{J}(\vec{x},t)\cdot(\vec{x}\cdot\nabla)\vec{A}_0(t) = \frac{1}{2}\int d^3x\, \frac{\partial\rho}{\partial t}\vec{x}\cdot(\vec{x}\cdot\nabla)\vec{A}_0(t) + \frac{1}{2}\int d^3x\, (\vec{x}\times\vec{J})\cdot(\nabla\times\vec{A}_0(t)). \quad (15)$$

Putting all the pieces together, we have

$$\begin{aligned} V(t) &= \int d^3x\, \left(\rho(\vec{x},t)\varphi(\vec{x},t) - \frac{1}{c}\vec{J}(\vec{x},t)\cdot\vec{A}(\vec{x},t)\right) \\ &= \int d^3x\, \rho(\vec{x},t)\left(\varphi_0(t) + \vec{x}\cdot\nabla\varphi_0(t) + \frac{1}{2}\vec{x}\vec{x}\cdot\nabla\nabla\varphi_0(t) + \cdots\right) \\ &\quad - \frac{1}{c}\int d^3x\, \frac{\partial\rho}{\partial t}\vec{x}\cdot\left(\vec{A}_0(t) + \frac{1}{2}(\vec{x}\cdot\nabla)\vec{A}_0(t) + \cdots\right) \\ &\quad - \frac{1}{2c}\int d^3x\, (\vec{x}\times\vec{J})\cdot(\nabla\times\vec{A}_0(t)) + \cdots. \end{aligned} \quad (16)$$

The unphysical long-range contribution to the excitation interaction of Ref. [9] can be traced to the term containing the time derivative of the charge density, $\partial\rho/\partial t$.

We would now like to eliminate the terms containing the time derivative of the charge density, $\partial\rho/\partial t$, in Eq. (16). We can do this by making the gauge transformation $\Lambda(\vec{x},t)$ given by the factor multiplying this term

$$\begin{aligned} \Lambda(\vec{x},t) &= -\vec{x}\cdot\left(\vec{A}_0(t) + \frac{1}{2}(\vec{x}\cdot\nabla)\vec{A}_0(t) + \cdots\right) \\ &= -\int_0^1 du\, \vec{x}\cdot\vec{A}(u\vec{x},t). \end{aligned} \quad (17)$$

The vector potential that results from the gauge transformation can be expanded as

$$\begin{aligned} \vec{A}'(\vec{x},t) &= \vec{A}(\vec{x},t) + \nabla\Lambda(\vec{x},t) \\ &= -\tfrac{1}{2}\vec{x}\times(\nabla\times\vec{A}_0) + \cdots, \end{aligned} \quad (18)$$

while the transformed scalar potential can be expanded as

$$\begin{aligned} \varphi'(\vec{x},t) &= \varphi(\vec{x},t) - \frac{1}{c}\frac{\partial\Lambda}{\partial t} \\ &= \varphi_0(t) + \vec{x}\cdot\left(\nabla\varphi_0(t) + \frac{1}{c}\frac{\partial\vec{A}_0}{\partial t}\right) \\ &\quad + \frac{1}{2}\vec{x}\vec{x}\cdot\nabla\left(\nabla\varphi_0(t) + \frac{1}{c}\frac{\partial\vec{A}_0}{\partial t}\right) + \cdots. \end{aligned} \quad (19)$$

We can then rewrite the interaction as

$$V(t) \approx \int d^3x\, \rho(\vec{x},t)\left(\varphi_0(t) + \vec{x}\cdot\left(\nabla\varphi_0(t) + \frac{1}{c}\frac{\partial\vec{A}_0}{\partial t}\right)\right.$$
$$\left. + \frac{1}{2}\vec{x}\vec{x}\cdot\nabla\left(\nabla\varphi_0(t) + \frac{1}{c}\frac{\partial\vec{A}_0}{\partial t}\right) + \cdots\right)$$
$$- \frac{1}{2c}\int d^3x\,(\vec{x}\times\vec{J})\cdot(\nabla\times\vec{A}_0(t)) + \cdots, \qquad (20)$$

which we can express in terms of the electromagnetic fields $\vec{E}_0$ and $\vec{B}_0$ at $\vec{x} = 0$ as

$$V(t) \approx \int d^3x\,\rho(\vec{x},t)\left(\varphi_0(t) - \vec{x}\cdot\vec{E}_0(t)\right.$$
$$\left. - \frac{1}{2}\vec{x}\vec{x}\cdot\nabla\vec{E}_0(t) + \cdots\right)$$
$$- \frac{1}{2c}\int d^3x\,(\vec{x}\times\vec{J})\cdot\vec{B}_0(t) + \cdots. \qquad (21)$$

If we assume as well that the field-producing charge does not overlap with the nuclear one, we can write the electric quadrupole term as

$$\vec{x}\vec{x}\cdot\nabla\vec{E}_0 = \sum_{i,j} x_i x_j \partial_j E_{0i}$$
$$= \sum_{i,j}(x_i x_j - \vec{x}^2\delta_{ij}/3)\partial_j E_{0i}, \qquad (22)$$

since, in that case, $\nabla\cdot\vec{E}_0 = 0$.

We can then write the interaction in a form that parallels the classical (Cartesian) multipole expansion [23], as

$$V(t) = q\varphi(t) - \vec{d}\cdot\vec{E}_0(t) - \frac{1}{2}\sum_{i,j} Q_{ij}\partial_j E_{0i}(t)$$
$$- \vec{m}\cdot\vec{B}_0(t) + \cdots, \qquad (23)$$

where q is the charge,

$$q = \int d^3x\,\rho(\vec{x},t), \qquad (24)$$

$\vec{d}$ is the electric dipole operator,

$$\vec{d} = \int d^3x\,\vec{x}\,\rho(\vec{x},t), \qquad (25)$$

the Q_{ij} are the traceless electric quadrupole operators,

$$Q_{ij} = \int d^3x\,(x_i x_j - \vec{x}^2\delta_{ij}/3)\,\rho(\vec{x},t), \qquad (26)$$

and $\vec{m}$ is the magnetic dipole operator,

$$\vec{m} = \frac{1}{2c}\int d^3x\,\vec{x}\times\vec{J}(\vec{x},t). \qquad (27)$$

The multipole expansion does not depend on whether we have included magnetization currents, exchange contributions or other corrections that determine the detailed structure of the target charge and current densities. The only property of these densities that we have used is the continuity equation, Eq. (11), which should be valid in any case.

The multipole expansion given here can be extended to all orders without great difficulty. It can be expressed compactly as

$$V(t) = q\varphi(t) - \int d^3x\,\rho(\vec{x},t)\,\vec{x}\cdot\int_0^1 du\,\vec{E}(u\vec{x},t)$$
$$- \frac{1}{c}\int d^3x\,(\vec{x}\times\vec{J})\cdot\int_0^1 du\,u\,\vec{B}(u\vec{x},t). \qquad (28)$$

It satisfies the gauge condition $\vec{x}\cdot\vec{A}(\vec{x},t) = 0$, which can be rewritten as

$$\int_0^1 du\,\vec{x}\cdot\vec{A}(u\vec{x},t) = 0, \qquad (29)$$

[see Eq. (17)] and is known as the multipolar or Poincaré gauge [20]. A drawback to our formulation is that it has been performed in a Cartesian rather than a spherical basis. However, the expansion in the spherical basis should be directly deducible from the Cartesian one, since the two are equivalent.

In the physically intuitive form given above, the electromagnetic interaction poses no problem, even when the excitation and decay of resonant states is considered. As an example, we take the Liénard-Wiechert potential due to a relativistic nucleus of charge Z passing on a straight-line trajectory with velocity v in the $\hat{z}$ direction at a distance b_0 from the center of the charge/current distribution of the target. We then have [23]

$$\varphi(\vec{b},z,t) = \gamma\frac{Ze}{\sqrt{(\vec{b}-\vec{b}_0)^2 + \gamma^2(z-vt)^2}}$$

and

$$\vec{A}(\vec{b},z,t) = \frac{v}{c}\hat{z}\,\varphi(\vec{b},z,t). \qquad (30)$$

The transverse and longitudinal components of the electric field, which induce dipole excitation, are

$$\vec{E}_{0\perp}(t) = -\gamma\vec{b}_0\frac{Ze}{\left(\vec{b}_0^2 + (\gamma vt)^2\right)^{3/2}}$$

and

$$E_{0||}(t) = -\gamma vt\frac{Ze}{\left(\vec{b}_0^2 + (\gamma vt)^2\right)^{3/2}}, \qquad (31)$$

and tend to zero as $b_0^{-2}$and b_0^{-3}, respectively, as the impact parameter increases. At high energies, the excitation is dominated by the transverse modes, which produce a cross section that grows as $\ln(b_{\max}/b_{\min})$, as expected [6].

Bayman and Zardi [24] have observed that the mixed representation of the interaction given in Ref. [9] neglects relativistic corrections to the quadrupole and higher multipole terms, which become important at high energies. These are included and discussed in their work and in Ref. [10]. They are also taken into account correctly (and automatically) when the pure field representation is used.

As mentioned earlier, Bayman and Zardi have also recently compared calculations of relativistic Coulomb excitation in the Lorentz and Coulomb gauges [11]. They find that the cross sections in the Lorentz gauge increases dramatically with respect to those in the Coulomb gauge at energies above about

2 GeV/nucleon. Although the Coulomb gauge is not equivalent to the one we present here, we suspect that it too might include only physical contributions to coupled-channels cross sections. We are of the opinion, however, that the optimal form of the interaction in such calculations is the one given here, in which the excitation interaction is expressed in terms of the physical fields and their derivatives.

We have shown that, through an appropriate gauge transformation, the Coulomb excitation component of the semiclassical form of the electromagnetic interaction can be expressed in terms of the electromagnetic fields and their derivatives. Aside from making a satisfying parallel with the classical case, the pure field representation of the excitation interaction, known as the multipolar or Poincaré gauge, provides physically reasonable cross sections, even when resonance excitation and decay is taken into account.

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