Eikonal approximation applied to many-electron atoms

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The scattering of electrons by target atoms with Q electrons is considered in the full eikonal approximation. An expression for the scattering amplitude is given which reduces the number of integrations from $3Q+3$ to $2Q$.

There has been a great deal of interest in applying the Glauber and eikonal approximations to problems in atomic physics.[1] Recently Gau and Macek showed that a compact expression for the full eikonal amplitude can be derived for the scattering of electrons by hydrogen atoms.[2] In this Comment we wish to point out that their technique can be extended to Q-electron atoms and this reduces the $(3Q+3)$-fold integration down to a $2Q$-fold integration.

The eikonal approximation to the scattering amplitude for electron excitation of an arbitrary Q-electron atom from its initial state i to its final state f is

$$F_{fi}(\vec{q}) = -\frac{2m}{4\pi\hbar^2}\int \exp(i\vec{q}\cdot\vec{R})V(R,R_j')\times\exp\left(-\frac{i}{\hbar v}\int_{-\infty}^{Z} V(R,R_j')\,dz\right)\times u_f^*(\vec{r}_1,\ldots,\vec{r}_Q)\times u_i(\vec{r}_1,\ldots\vec{r}_Q)\,d\vec{R}\,d\vec{r}_1\cdots d\vec{r}_Q\,, \tag{1}$$

where $\vec{R}$ and $\vec{r}_j$ are the coordinates (relative to the nucleus) of the incident and the jth bound electron, respectively, $\vec{R}_j'=\vec{R}-\vec{r}_j$, $m\vec{v}=\hbar\vec{k}$ is the incident electron's momentum, $\vec{q}=\vec{k}-\vec{k}'$ is the momentum transfer to the target, and u_f and u_i are the final and initial bound states of the target atom. Here $\vec{k}$ is along the z axis, and the interaction potential is

$$V(R,R_j') = e^2\sum_{j=1}^{Q}\left(\frac{1}{R_j'}-\frac{1}{R}\right). \tag{2}$$

The eikonal phase in Eq. (1) can be evaluated to give

$$\exp\left(-\frac{i}{\hbar v}\int_{-\infty}^{Z} V(R,R_j')\,dz\right) = \prod_{j=1}^{Q}\frac{(R_j'-Z_j')^{i\eta}}{(R-Z)^{i\eta Q}}\,, \tag{3}$$

where $\eta = e^2/\hbar v$.

In order to evaluate Eq. (1) for an arbitrary Q-electron atom, we assume that the product of the bound-state wave functions has the form[3]

$$u_f^*(\vec{r}_1,\ldots,\vec{r}_Q)u_i(\vec{r}_1,\ldots,\vec{r}_Q) = \sum_{k=0}^{N} c_k\left(\prod_{j=1}^{Q}\left[r_j^{n_{kj}}e^{-\mu_{kj}r_j}Y^*_{l_j'm_j'}(\theta_j,\phi_j)Y_{l_jm_j}(\theta_j,\phi_j)\right]\right). \tag{4}$$

It can be shown that the above wave-function product $u_f^*u_i$ can be written as

$$u_f^*(\vec{r}_1,\ldots,\vec{r}_Q)u_i(\vec{r}_1,\ldots,\vec{r}_Q) = \sum_{k=0}^{N} c_k\left(\prod_{j=1}^{Q}\mathfrak{D}_{kj}f_{kj}(\vec{r}_j)\right)_{\vec{\gamma}_j=0}, \tag{5}$$

where

$$f_{kj}(\vec{r}_j) = \exp(-\mu_{kj}r_j + i\vec{\gamma}_j\cdot\vec{r}_j)\,. \tag{6}$$

The differential operators $\mathfrak{D}_{kj}$ which generate the required wave functions are given by

$$\mathfrak{D}_{kj} = \mathfrak{D}(n_{kj}, l_j, m_j, \mu_{kj}, \vec{\gamma}_j)\mathfrak{D}(n_{kj}, l_j', m_j', \mu_{kj}, -\vec{\gamma}_j)\,, \tag{7a}$$

$$\mathfrak{D}(n,l,m,\mu,\pm\vec{\gamma}) = \frac{(-1)^m}{2^l}\left(\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}\right)^{1/2}D^m(\pm\vec{\gamma})\times\sum_{P=0}^{[(l-m)/2]}\frac{(-1)^P(2l-2P)!}{P!(l-P)!(l-2P-m)!}\times D^{2P-l+n/2}(\mu)D^{l-2P-m}(\gamma_z)\,, \tag{7b}$$

where

$$D(\mu) = -\frac{\partial}{\partial\mu}\,,\quad D(\pm\vec{\gamma}) = -i\left(\frac{\partial}{\partial\gamma_x}\pm i\frac{\partial}{\partial\gamma_y}\right),\quad D(\gamma_z) = -i\frac{\partial}{\partial\gamma_z}\,. \tag{7c}$$

In the upper limit of the sum, $[a]$ denotes the largest integer contained in a. Note that since $\mathfrak{D}$ contains the term $D^{2P-l+n/2}(\mu)$, it makes sense only in the product of Eq. (7a) if n is odd.

Inserting the eikonal phase given by Eq. (3) and the wave functions given by Eq. (5) into Eq. (1), the scattering amplitude becomes

$$F_{fi}(\vec{q})=\frac{-1}{2\pi a_0}\int \frac{e^{i\vec{q}\cdot\vec{R}}}{(R-Z)^{i\eta Q}}\sum_{s=1}^{Q}\left(\frac{1}{R_s'}-\frac{1}{R}\right)\prod_{j'=1}^{Q}(R_{j'}'-Z_{j'}')^{i\eta}\left[\sum_{k=0}^{N}c_k\left(\prod_{j=1}^{Q}\mathfrak{D}_{kj}f_{kj}(\vec{r}_j)\right)\right]d\vec{R}\,d\vec{r}_1\cdots d\vec{r}_Q\Big|_{\vec{\gamma}_j=0}. \tag{8}$$

The above expression can be rewritten as

$$F_{fi}(q)=-\frac{1}{2\pi a_0}\sum_{k=0}^{N}c_k\int\frac{e^{i\vec{q}\cdot\vec{R}}\,d\vec{R}}{(R-Z)^{i\eta Q}}\sum_{s=1}^{Q}\mathfrak{D}_{ks}\left(\frac{1}{R_s'}-\frac{1}{R}\right)(R_s'-Z_s')^{i\eta}f_{ks}(\vec{r}_s)\,d\vec{r}_s$$
$$\times\left(\prod_{\substack{j=1\\ j\neq s}}^{Q}\mathfrak{D}_{kj}\int(R_j'-Z_j')^{i\eta}f_{kj}(\vec{r}_j)\,d\vec{r}_j\right)\Big|_{\vec{\gamma}_j=\vec{\gamma}_s=0}. \tag{9}$$

To proceed with the reduction of Eq. (9), we follow the technique of Gau and Macek. We use the definition of the γ function[4] to write

$$(R'-Z')^{i\eta}=[\Gamma(-i\eta)]^{-1}\int_0^\infty d\lambda\,\lambda^{-i\eta-1}e^{-\lambda(R'-Z')}. \tag{10}$$

Substituting Eq. (10) into Eq. (9) and taking the Fourier transforms of the factors containing R_s' and R_j' allows the $\vec{r}_s$ and $\vec{r}_j$ integrations to be done; performing these integrations results in the following expression for $F_{fi}(\vec{q})$:

$$F_{fi}(\vec{q})=\frac{-2^Q}{2\pi[\Gamma(-i\eta)]^Q\pi^Q a_0}\sum_{k=0}^{N}c_k\int\frac{e^{i\vec{q}\cdot\vec{R}}d\vec{R}}{(R-Z)^{i\eta Q}}\sum_{s=1}^{Q}\mathfrak{D}_{ks}\int_0^\infty d\lambda_s\,\lambda_s^{-i\eta-1}$$
$$\times\left[-\frac{\partial}{\partial\mu_{ks}}\int\frac{e^{i\vec{k}_s\cdot\vec{R}}\,d\vec{k}_s}{\mu_{ks}^2+(\vec{k}_s-\vec{\gamma}_s)^2}\left(\frac{1}{(k_s^2+2i\lambda_s k_{sz})}-\frac{2\lambda_s}{R}\frac{1}{(k_s^2+2i\lambda_s k_{sz})^2}\right)\right]$$
$$\times\prod_{\substack{j=1\\ j\neq s}}^{Q}\mathfrak{D}_{kj}\int_0^\infty d\lambda_j\,\lambda_j^{-i\eta}\left(2\frac{\partial}{\partial\mu_{kj}}\int\frac{e^{i\vec{k}_j\cdot\vec{R}}\,d\vec{k}_j}{[\mu_{kj}^2+(\vec{k}_j-\vec{\gamma}_j)^2](k_j^2+2i\lambda_j k_{jz})^2}\right)\Big|_{\vec{\gamma}_j=\vec{\gamma}_s=0}. \tag{11}$$

The integrals over $d\vec{k}_s$ and $d\vec{k}_j$ may now be done using the Feynman parametrization technique. The result is

$$F_{fi}(\vec{q})=\frac{-(2\pi)^{Q-1}2^{2Q}}{a_0[\Gamma(-i\eta)]^Q}\sum_{k=0}^{N}c_k\int\frac{e^{i\vec{q}\cdot\vec{R}}d\vec{R}}{R(R-Z)^{i\eta Q}}\sum_{s=1}^{Q}\mathfrak{D}_{ks}\mu_{ks}\left(\frac{\partial}{\partial\mu_{ks}^2}\right)^2\left[\int_0^\infty d\lambda_s\,\lambda_s^{-i\eta-1}\int_0^1 d\chi_s\,\chi_s^{-1}e^{i\vec{\alpha}_s\cdot\vec{R}-\Lambda_{ks}R}\left(1-\frac{\lambda_s(1-\chi_s)}{\Lambda_{ks}}\right)\right]$$
$$\times\prod_{\substack{j=1\\ j\neq s}}^{Q}\mathfrak{D}_{kj}\mu_{kj}\left(\frac{\partial}{\partial\mu_{kj}^2}\right)^2\left(\int_0^\infty d\lambda_j\,\lambda_j^{-i\eta}\int_0^1 d\chi_j\,\chi_j^{-1}(1-\chi_j)\Lambda_{kj}^{-1}e^{i\vec{\alpha}_j\cdot\vec{R}-\Lambda_{kj}R}\right)\Big|_{\vec{\gamma}_j=\vec{\gamma}_s=0}, \tag{12}$$

where Λ_{kj} and $\vec{\alpha}_j$ are defined by

$$\Lambda_{kj}=[\lambda_j^2(1-\chi_j)^2+2i\lambda_j\chi_j(1-\chi_j)\gamma_{jz}+\mu_{kj}^2\chi_j+\gamma_j^2\chi_j(1-\chi_j)]^{1/2}, \tag{13a}$$

$$\vec{\alpha}_j=\chi_j\vec{\gamma}_j-i\lambda_j(1-\chi_j)\hat{z}. \tag{13b}$$

The $\vec{R}$ integration in Eq. (12) may be performed by using parabolic coordinates[5]; this integral is

$$I_R=\int\frac{e^{i\vec{q}\cdot\vec{R}+i\vec{\alpha}\cdot\vec{R}-\Lambda_k R}\,d\vec{R}}{R(R-Z)^{i\eta Q}}=\pi 2^{2-i\eta Q}\,\Gamma(1-i\eta Q)\frac{(\Lambda_k^2+q'^2)^{i\eta Q-1}}{(\Lambda_k-iq_z')^{i\eta Q}}, \tag{14}$$

where

$$\Lambda_k=\sum_{j=1}^{Q}\Lambda_{kj},\quad \vec{q}\,'=\vec{q}+\vec{\alpha}=\vec{q}+\sum_{j=1}^{Q}\vec{\alpha}_j.$$

Inserting the above result into Eq. (12) results in the desired reduction of the scattering amplitude:

$$F_{fi}(\vec{q}) = -\frac{(2\pi)^Q 2^{2Q+1-i\eta Q}}{a_0}\frac{\Gamma(1-i\eta Q)}{[\Gamma(-i\eta)]^Q}\sum_{k=0}^{N} c_k \sum_{s=1}^{Q}\prod_{j=1}^{Q}\bigg[\mathfrak{D}_{kj}\mu_{kj}\left(\frac{\partial}{\partial\mu_{kj}^2}\right)^2\int_0^\infty d\lambda_j\,\lambda_j^{-i\eta-1}\int_0^1 d\chi_j\,\chi_j^{-1}$$
$$\times[\mathfrak{F}_{kj}(\delta_{js}, 1-\delta_{js}, 0, 1-\delta_{js}) - \mathfrak{F}_{kj}(\delta_{js}, 1, 0, 1)]\bigg]_{\vec{\gamma}_j=\vec{\gamma}_s=0}, \tag{15a}$$

where

$$\mathfrak{F}_{kj}(m,p,r,s) = \lambda_j^s(1-\chi_j)^s\Lambda_{kj}^{-p}(\Lambda_k^2+q'^2)^{i\eta-m}(\Lambda_k - iq_z')^{-i\eta-r}. \tag{15b}$$

Thus, the $(3Q+3)$-dimensional integral for the scattering amplitude has been reduced to a $2Q$-dimensional one. Note that for $Q=1$, which corresponds to a one-electron atom, our expression reduces to that of Gau and Macek,[2] which was derived by them for electron scattering by hydrogen atoms.

Although the tractability of our scattering amplitude has yet to be demonstrated, it may prove useful for calculations involving light atoms such as helium, or atoms in which the inner-shell electrons may be regarded as part of an inert core. The expression may be further generalized to include configuration wave functions if we let $l_j m_j \to l_{kj} m_{kj}$ and $l_j' m_j' \to l_{kj}' m_{kj}'$ in Eq. (4).

[1]The following references are intended to serve as a guide to the literature on the Glauber approximation and its application to atomic physics problems: R. J. Glauber, in *Lectures in Theoretical Physics*, edited by W. E. Brittin *et al.* (Interscience, New York, 1959); V. Franco, Phys. Rev. Lett. 20, 709 (1968); H. Tai, R. H. Bassel, E. Gerjuoy, and V. Franco, Phys. Rev. A 1, 1819 (1970); V. Franco, Phys. Rev. A 1, 1705 (1970); V. Franco, Phys. Rev. Lett. 26, 1088 (1971); B. K. Thomas and E. Gerjuoy, J. Math. Phys. 12, 1567 (1971); F. W. Byron, Jr., Phys. Rev. A 4, 1907 (1971); C. J. Joachain and M. H. Mittleman, Phys. Rev. A 4, 1492 (1971); W. Williamson, Jr., Aust. J. Phys. 25, 643 (1972); J. C. Y. Chen, C. J. Joachain, and K. M. Watson, Phys. Rev. A 5, 2460 (1972); A. C. Yates and A. Tenney, Phys. Rev. A 6, 1451 (1972); A. N. Tripathi, K. C. Mathur, and S. K. Joshi, J. Chem. Phys. 58, 1384 (1973); J. H. McGuire, M. G. Hidalgo, G. D. Doolen, and J. Nuttall, Phys. Rev. A 7, 973 (1973); H. R. J. Walters, J. Phys. B 6, 1003 (1973); B. K. Thomas and F. T. Chan, Phys. Rev. A 8, 252 (1973); F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. A 8, 1267 (1973); L. Hambro, J. C. Y. Chen, and T. Ishihara, Phys. Rev. A 8, 1283 (1973); J. C. Y. Chen, T. Ishihara, V. H. Ponce, and K. M. Watson, Phys. Rev. A 8, 1334 (1973); T. N. Chang, R. T. Poe, and P. Ray, Phys. Rev. Lett. 31, 1097 (1973); F. T. Chan and S. T. Chen, Phys. Rev. A 8, 2191 (1973); B. C. Saha, K. Sarkar, and A. S. Ghosh, J. Phys. B 6, 2303 (1973); J. C. Y. Chen, J. Phys. B 6, L351 (1973); V. Franco, Phys. Rev. A 8, 2927 (1973); F. W. Byron, Jr., Phys. Rev. A 8, 3266 (1973); J. Z. Terebey, J. Phys. B 7, 460 (1974); R. H. Shields and J. L. Peacher, Phys. Rev. A 9, 743 (1974); K. C. Mathur, Phys. Rev. A 9, 1220 (1974); J. E. Golden and J. H. McGuire, Phys. Rev. Lett. 32, 1218 (1974); J. L. Preacher and R. H. Shields, Phys. Rev. Lett. 9, 2371 (1974); F. T. Chan and S. T. Chen, Phys. Rev. A 9, 2393 (1974); F. W. Byron, Jr. and C. J. Joachain, Phys. Rev. A 9, 2559 (1974).

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