Barkas effect in a central collision: Exact numerical results and the tenth-order Born series

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The time-dependent Schrödinger equation for a central collision between a heavy point charge and a harmonically bound electron is solved numerically. This is done in a basis of energy eigenfunctions of the undisturbed electron. Our numerical method also provides the coefficients of the Born series for the collision. We compare the Born expansion with the exact results. In agreement with other calculations we find a significant Barkas effect for some collision parameter values. At low velocities the Barkas correction is shown to be very large, but at higher velocities it becomes very small even for ions with high charges.

I. INTRODUCTION

The slowing down of a fast charged particle in matter is mainly due to the inelastic Coulomb collisions with the bound electrons in the target. Conventionally, these inelastic processes are treated within the Bethe-Bloch formalism, where the distant collisions (with small momentum transfers) are treated within first-order perturbation theory, and the close collisions (with large momentum transfers) are considered to be free. Under the assumption that the projectile velocity is much larger than the mean orbital velocity of the target electrons, the well-known Bloch formula yields for the electronic stopping cross section in the nonrelativistic case[1]

$$S=\frac{4\pi(Z_1e^2)e^2}{mv^2}Z_2\left[\ln\left[\frac{2mv^2}{I}\right]+\psi(1)-\mathrm{Re}\psi\left[1+i\frac{Z_1e^2}{\hbar v}\right]\right]. \quad (1)$$

Here, Z_1 and v are projectile charge number and velocity, m and $-e$ are the electron mass and charge, and Z_2 and I are the atomic number and mean excitation potential of the target.

The Bloch formula is not the result of a perturbation expansion in the primary interaction between the projectile and the target electrons as is seen from the presence of $Z_1e^2/\hbar v$ in the last term. This term containing the ψ function is a close-collision correction, which stems from an exact treatment of the near singular part of free Rutherford scattering. Only for $|Z_1e^2/\hbar v|<1$ does the ψ function allow for expansion in $(Z_1e^2/\hbar v)^2$ yielding

$$\psi(1)-\mathrm{Re}\psi\left[1+i\frac{Z_1e^2}{\hbar v}\right]=\sum_{n=1}^{\infty}(-1)^n\zeta(2n+1)\times\left[\frac{Z_1e^2}{\hbar v}\right]^{2n}, \quad (2)$$

where $\zeta(n)$ is Riemann's ζ function. In the limit of $|Z_1e^2/\hbar v|\ll 1$ the stopping cross section therefore reduces to the Bethe formula[2]

$$S=\frac{4\pi(Z_1e^2)e^2}{mv^2}Z_2\ln\left[\frac{2mv^2}{I}\right], \quad (3)$$

which is the lowest term in a Born-series expansion in $Z_1e^2/\hbar v$. In the opposite limit of $Z_1e^2/\hbar v\gg 1$, Bohr's classical result is obtained:[3]

$$S=\frac{4\pi(Z_1e^2)e^2}{mv^2}Z_2\ln\left[\frac{1.123mv^3}{|Z_1|e^2\omega}\right]. \quad (4)$$

The Bloch formula thus directly reflects the transition from a quantal perturbative regime $|Z_1e^2/\hbar v|\ll 1$ to a classical nonperturbative one $|Z_1e^2/\hbar v|\gg 1$.[4]

A characteristic feature of the Bloch formula is that it is an even function in Z_1, i.e., invariant to the sign of the projectile charge. Experiments have shown, however, that sign-dependent processes do occur in the slowing down of fast charged particles. This was first shown by Barkas and co-workers by comparing the ranges of pions of opposite charge.[5] Later, the effect was confirmed and quantified,[6] most recently in precise measurements of the stopping of protons and antiprotons.[7]

The origin of this so-called Barkas effect has been sought in the polarization of the target atom by the penetrating projectile. In the presence of a nonvanishing binding force on the electrons, this will give rise to uneven terms in the Born series. The Barkas effect has been attributed to the leading uneven term in this series, i.e., the Z_1^3 term.

In the first theoretical account of the Z_1^3 term (the Barkas term), it was claimed that only distant collisions would contribute to the effect.[8] Later, however, it was argued that a roughly equal contribution would come from the close collisions.[9] This assertion has been confirmed by recent quantitative calculations.[10–13]

The presence of this sign-dependent effect shows that

the binding cannot be neglected even for the close collisions. In fact, inclusion of the binding may affect the close-collision part of all terms (even and odd) of the Born series at least at moderate and low velocities, where the collision time is sufficiently long for the target electron to probe its binding potential during the collision. This is important since the close collisions play a crucial role for the difference between the stopping formulas considered above.

In order to investigate the importance of binding in close collisions, we consider the idealized case of a central collision of a heavy charged particle with a harmonically bound electron. For this system, we first calculate the energy transfer to the oscillator numerically and, second, to tenth order in the Born series.

The choice of a harmonic binding potential allows for easy evaluation of the matrix elements and direct comparison with previous results for the Z_1^2 term,[14] the Z_1^3 term,[11] and the Z_1^4 term.[15] Our numerical method, however, is sufficiently general to cover also more realistic atomic potentials.

The case of a central collision, i.e., a collision with impact parameter zero, is of special interest, since the deviations from the perturbative results are expected to be particularly pronounced in this limit. Furthermore, the cylindric symmetry of a central collision reduces the problem by one spatial degree of freedom while retaining the complexity that a close collision may present. This serves to reduce the required computation times.

We plan to return to the general collision in a future publication.

II. BASIC EQUATIONS

We consider a massive point charge $Z_1 e$ moving along a classical trajectory passing through a target atom consisting of an electron with charge $-e$ bound harmonically with a resonance frequency ω.

Initially, the harmonic oscillator is assumed to be in its ground state $|0\rangle$ defined by

$$H_0|n\rangle = E_n|n\rangle \ , \tag{5}$$

where H_0 is the Hamiltonian of an unperturbed oscillator, E_n is the energy corresponding to the eigenstate $|n\rangle$, and $n=0,1,2,\ldots$. During the collision, the oscillator is excited by the time-dependent Coulomb potential

$$V(t)=\frac{-Z_1 e^2}{|\mathbf{r}-\mathbf{R}(t)|} \ , \tag{6}$$

where $\mathbf{r}$ and $\mathbf{R}(t)$ define the positions of the bound electron and the projectile, respectively.

The collision process is described by the time-dependent Schrödinger equation for the oscillator. In the interaction picture, this equation is given by

$$i\hbar\frac{d}{dt}\tilde{\Psi}(t)=\tilde{V}(t)\tilde{\Psi}(t) \ . \tag{7}$$

Here, $\tilde{\Psi}(t)=e^{iH_0 t/\hbar}\Psi(t)$, with $\Psi(t)$ being the wave function of the oscillator, and $\tilde{\Psi}(t)=e^{iH_0 t/\hbar}V(t)e^{-iH_0 t/\hbar}$. By expanding $\tilde{\Psi}(t)$ in terms of the unperturbed energy eigenfunctions of the oscillator

$$\tilde{\Psi}(t)=\sum_n c_n(t)|n\rangle \tag{8}$$

the mean energy transfer ΔE is given by

$$\Delta E=\sum_n |c_n(\infty)|^2(E_n-E_0) \ . \tag{9}$$

Generally, ΔE will depend on the impact parameter of the projectile in the collision. The overall stopping cross section is given by

$$S=2\pi\int_0^\infty dp\,\Delta E(p)p \ , \tag{10}$$

where p is the impact parameter. In the present paper we consider only the energy transfer in a central collision, i.e., $\Delta E=\Delta E(p=0)$.

Equation (7) can be transformed to an integral equation, and assuming that the interaction $\tilde{V}(t)$ is weak throughout the collision it can be solved iteratively by standard methods of quantal perturbation theory.[16] This yields c_n as an expansion in $Z_1 e^2/\hbar v$,

$$c_n=\delta_{n0}+c_n^{(1)}+c_n^{(2)}+c_n^{(3)}+\cdots \ . \tag{11}$$

By combining these probability amplitudes in the appropriate way, the corresponding expansion for ΔE follows from substitution in (11):

$$\Delta E=\Delta E^{(2)}+\Delta E^{(3)}+\Delta E^{(4)}+\cdots \ . \tag{12}$$

The terms up to $\Delta E^{(4)}$ have recently been evaluated as a limiting case in more general treatments concerning the full impact parameter dependence of the energy transfer.[11,14,15] Extension of these calculations to even higher order is complicated by the increasing number of intermediate states needed. In practice, this kind of calculation is therefore restricted to the first few terms. Furthermore, in a central collision we cannot assume that the interaction is weak and a Born series expansion is therefore of little use.

In order to overcome these difficulties, we propose an alternative numerical method for solving Eq. (7).

Integration of (7) from a time t_j to time t_{j+1} gives

$$\tilde{\Psi}(t_{j+1})=\tilde{\Psi}(t_j)+\frac{1}{i\hbar}\int_{t_j}^{t_{j+1}}dt\tilde{V}(t)\tilde{\Psi}(t) \ . \tag{13}$$

Irrespective of the strength of the interaction $\tilde{V}(t)$, its contribution in (13) is small for $\Delta t=t_{j+1}-t_j$ sufficiently small. We use this fact to expand the integrand in (13) in powers of Δt and truncate the series after the second term. This truncation introduces an error in (13) of $O(\Delta t^3)$. Consequently, the result of using (13) repeatedly to find $\tilde{\Psi}(t_{\max})$ from $\tilde{\Psi}(t_{\min})$ contains an error of $O(\Delta t^2)$. Here, $t_{\min}$ and $t_{\max}$ are times chosen so that the collision process is truncated well outside several adiabatic distances.[4] In principle we can make this error arbitrarily small by choosing Δt small. In practice a limit is set by errors caused by a cutoff in energy, introduced below, and execution time requirements. For the present, we notice that the global error is $O(\Delta t^2)$. Hence, by doubling the number of timesteps between $t_{\min}$ and $t_{\max}$ and thereby the execution time, we can quadruple the numerical

precision. This tradeoff makes the method practically useful.

A heavy projectile with velocity v can at most transfer an energy $2mv^2$ to a free electron at rest. When the zero-point motion due to the binding is taken into account, more energy can be transferred. However, for a harmonic oscillator $2mv^2/\hbar\omega$ defines an approximate cutoff in the number of energy eigenstates required to give a full quantal description of the collision.

This finite set of eigenfunctions provide a natural discretization of the collision process. In the following we describe two ways to expand (13) to second order in Δt and solve (7) within this basis.

A. Method I

By approximating $\tilde{\Psi}(t)$ linearly through $\tilde{\Psi}(t_{j-1})$ and $\tilde{\Psi}(t_j)$ for $t_j \le t \le t_{j+1}$ and inserting this in (13), we get

$$\tilde{\Psi}(t_{j+1})=\tilde{\Psi}(t_j)+\frac{1}{i\hbar}\int_{t_j}^{t_{j+1}}dt\,\tilde{V}(t)\left[\tilde{\Psi}(t_j)+[\tilde{\Psi}(t_j)-\tilde{\Psi}(t_{j-1})]\frac{t-t_j}{\Delta t}\right]+O(\Delta t^3)\ . \tag{14}$$

Using (8) we find

$$c_m(t_{j+1})=c_m(t_j)+\frac{1}{i\hbar}\sum_{|n|\le n_{\max}}\int_{t_j}^{t_{j+1}}dt\,e^{i(E_m-E_n)t/\hbar}\langle m|V(t)|n\rangle\left[c_n(t_j)+[c_n(t_j)-c_n(t_{j-1})]\frac{t-t_j}{\Delta t}\right]\ . \tag{15}$$

In (15) we have explicitly introduced a cutoff $n_{\max}$ in the energy, hence in the number of eigenstates used to describe the collision process. By $|n|$ is meant $|n_x+n_y+n_z|$, where $n=(n_x,n_y,n_z)$ are the energy quantum numbers of the harmonic oscillator in three dimensions. With $n_{\max}$ in place the integrand in (15) can be Taylor expanded about $t_{j+1/2}=(t_j+t_{j+1})/2$ and the integration carried out. That leaves us with

$$c_m(t_{j+1})=c_m(t_j)+\frac{\Delta t}{i\hbar}\sum_{|n|\le n_{\max}}e^{i(E_m-E_n)t_{j+1/2}/\hbar}\langle m|V(t_{j+1/2})|n\rangle[\tfrac{3}{2}c_n(t_j)-\tfrac{1}{2}c_n(t_{j-1})]\ , \tag{16}$$

which provides a method for approximate solution of Eq. (7). Note that the method is formally very similar to the two-step Adams-Bashforth method for the solution of ordinary differential equations, except that we have used the linearity of the Schrödinger equation to evaluate $V(t)$ at midpoints between the points in time where $\tilde{\Psi}(t)$ is evaluated.

B. Method II

Iterating (13) once, we have

$$\tilde{\Psi}(t_{j+1})=\tilde{\Psi}(t_j)+\frac{1}{i\hbar}\int_{t_j}^{t_{j+1}}dt\,\tilde{V}(t)\tilde{\Psi}(t_j)-\frac{1}{\hbar^2}\int_{t_j}^{t_{j+1}}dt\int_{t_j}^{t}dt'\tilde{V}(t)\tilde{V}(t')\tilde{\Psi}(t_j)+O(\Delta t^3)\ . \tag{17}$$

Again we assume that only the states $|n|\le n_{\max}$ are excited, and Taylor expand the time dependence around $t_{j+1/2}$. That leaves us with a one-step formula

$$\begin{aligned}c_m(t_{j+1})=c_m(t_j)&+\frac{\Delta t}{i\hbar}\sum_{|n|\le n_{\max}}e^{i(E_m-E_n)t_{j+1/2}/\hbar}\langle m|V(t_{j+1/2})|n\rangle c_n(t_j)\\&-\frac{(\Delta t)^2}{\hbar^2}\sum_{|n|\le n_{\max}}e^{i(E_m-E_n)t_{j+1/2}/\hbar}\langle m|V^2(t_{j+1/2})|n\rangle c_n(t_j)\ .\end{aligned} \tag{18}$$

As method II involves the evaluation of two matrix elements in each time step, it is less efficient than method I as long as $\tilde{\Psi}(t)$ does not change rapidly with t. When it does, the one-step method in (18) reproduces this change more effectively than the two-step method in (16).

Both methods are easily adapted to find many coefficients of the Born series for the collision process. This is done by introducing $c_m^{(k)}(t_j)$, the coefficient of the kth-order term in the perturbation expansion of $c_m(t_j)$. When c_m is written as $\sum_k c_m^{(k)}(Z_1e^2/\hbar v)^k$ in (18), it follows that

$$\begin{aligned}c_m^{(k)}(t_{j+1})=c_m^{(k)}(t_j)&+\frac{\Delta t}{i\hbar}\sum_{|n|\le n_{\max}}e^{i(E_m-E_n)t_{j+1/2}/\hbar}\langle m|V(t_{j+1/2})|n\rangle c_n^{(k-1)}(t_j)\\&-\frac{(\Delta t)^2}{\hbar^2}\sum_{|n|\le n_{\max}}e^{i(E_m-E_n)t_{j+1/2}/\hbar}\langle m|V^2(t_{j+1/2})|n\rangle c_n^{(k-2)}(t_j)\ .\end{aligned} \tag{19}$$

Iteration of the recursion relations (18) from the initial condition $c_m^{(k)}(t_{\min})=\delta_{k,0}\delta_{m,0}$ gives $c_m^{(k)}(t_{\max})$. From these coefficients other Born series are derived, for example that in (12). A two-step expression similar to (19) can be derived from (16).

Our numerical method of solution of (7) is related to the close-coupling scheme, which is commonly used in similar problems.[17,18] It differs, however, from these calculations by the use of a large set of eigenfunctions determined by a physical cutoff. By a proper choice of $n_{\max}$ the error due to the finite size of the basis can therefore be made arbitrarily small.

The discretization in energy eigenfunctions in (16) and (18) differs distinctly from the discretization on a spatial lattice used in standard models for parabolic differential equations. When we compare these methods we see that our transfer matrix is dense as opposed to the sparse transfer matrix for the lattice discretization. Because of the naturalness of our discretization and cutoff, our transfer matrix is smaller. This property and the expression of the matrix elements given below ensure that our method works. It is, however, no general alternative to established methods, since it is practical only when (5) can be solved analytically.

III. EVALUATION

So far our derivations have been quite general in the sense that we have only assumed that H_0 is integrable and that the projectile follows a classical trajectory specified by $\mathbf{R}(t)$. In the following we assume that the projectile moves uniformly with velocity v along a straight-line trajectory passing through the center of a harmonic oscillator target. We thus do not take into account the Coulomb deflection on the nucleus that will take place in a realistic atomic collision. In the energy region considered in this paper, however, the effect of the Coulomb deflection is negligible except for the very heaviest targets.

In the calculation we use cylindric coordinates with the oscillator placed at the origin and the axis of symmetry along the trajectory of the projectile. In this system the position of the oscillator and the point charge are given by $\mathbf{r}=(z,r,\phi)$ and $\mathbf{R}(t)=(vt,0,0)$, respectively. By symmetry the ϕ coordinate drops out of the calculation and the allowed transitions of the oscillator are therefore characterized only by the axial and radial quantum numbers

$$|\nu l\rangle=|\nu\rangle|l\rangle\ , \tag{20}$$

where

$$|\nu\rangle=\left[\frac{\beta}{\sqrt{\pi}\nu!2^{\nu}}\right]^{1/2}\mathrm{H}_{\nu}(\beta z)e^{-\beta^2z^2/2} \tag{21}$$

and

$$|l\rangle=\beta\left[\frac{2l!}{l!}\right]^{1/2}\mathrm{L}_l(\beta^2r^2)e^{-\beta^2r^2/2}\ . \tag{22}$$

H_{ν} and L_l are Hermite and Laguerre polynomials and $\beta=\sqrt{m\omega/\hbar}$. The corresponding energy levels are given by

$$E_{\nu l}=(\nu+2l+\tfrac{3}{2})\hbar\omega\ . \tag{23}$$

The matrix elements $\langle\mu k|V(t)|\nu l\rangle$ occurring in (16) and (18) have been evaluated in (11) yielding

$$\langle\mu k|V(t)|\nu l\rangle=-\frac{Z_1e^2\beta}{\sqrt{\pi}}\int_0^1 d\sigma\,\sigma^{-1/2}B^z_{\mu\nu}(\sigma,vt)\times B^r_{kl}(\sigma,0)\ , \tag{24}$$

where

$$B^z_{\mu\nu}(\sigma,vt)=e^{-\sigma\beta^2v^2t^2}\times\sum_{j=0}^{\min(\mu,\nu)}\frac{(\mu!\nu!)^{1/2}}{j!(\mu-j)!(\nu-j)!}\times\left[\frac{\sigma}{2}\right]^{(\mu+\nu-2j)/2}\times\mathrm{H}_{\mu+\nu-2j}(\sigma^{1/2}\beta vt) \tag{25}$$

and

$$B^r_{kl}(\sigma,0)=\sigma^{k+l}\sum_{i=0}^{\min(k,l)}\frac{(k+l-i)!}{i!(l-i)!(k-i)!}\left[\frac{1-2\sigma}{\sigma^2}\right]^i\ . \tag{26}$$

The matrix elements $\langle\mu k|V^2(t)|\nu l\rangle$, which are needed only in (18), can be evaluated similarly:

$$\langle\mu k|V^2(t)|\nu l\rangle=(Z_1e^2\beta)^2\int_0^1 d\sigma(1-\sigma)^{-1/2}\times B^z_{\mu\nu}(\sigma,vt)B^r_{kl}(\sigma,0)\ . \tag{27}$$

The integrals over σ in (24) and (27) allow for easy numerical evaluation by Gauss-Legendre quadrature, thus enabling us to integrate (7) in some fixed interval. We choose the initial and final position of the projectile to be $\beta vt=-20.0$ and $\beta vt=20.0$, which for $2mv^2/\hbar\omega\leq 100$ is well outside several adiabatic distances.

The choice of steplength Δt and cutoff value for the number of oscillator eigenstates $n_{\max}$ depends strongly on the actual parameters characterizing the problem. The pertinent dimensionless variables in the collision are $Z_1e^2/\hbar v$ and $\hbar\omega/2mv^2$. While $Z_1e^2/\hbar v$ can be interpreted as the effective strength of the interaction between the projectile and the bound electron, $\hbar\omega/2mv^2$measures the importance of the binding force during the collision. For a large value of $Z_1e^2/\hbar v$ a small steplength Δt is required. Conversely, the choice of $n_{\max}$ is mainly determined by $\hbar\omega/2mv^2$ through the cutoff in the number of energy eigenstates discussed above. The largest cutoff values needed in the calculation was $n_{\max}=52$ corresponding to a basis of 729 oscillator eigenstates. The computing required in this case was approximately 1 h on the Danish Amdahl VP1100 vector facility.

We have arranged for an overall accuracy of about 1% for all values of $Z_1e^2/\hbar v$ and $\hbar\omega/2mv^2$.

IV. RESULTS

The mean energy transfer in a central collision is conveniently expressed through the dimensionless quantity $\tilde{T}$ defined by

$$\Delta E = \left[\frac{Z_1e^2}{\hbar v}\right]^2 \hbar\omega\tilde{T} , \tag{28}$$

where $\tilde{T}$ in general depends both on $Z_1e^2/\hbar v$ and $\hbar\omega/2mv^2$. By expanding $\tilde{T}$ in powers of $Z_1e^2/\hbar v$ we get the Born series.

$$\tilde{T} = \tilde{T}_0 + \tilde{T}_1\left[\frac{Z_1e^2}{\hbar v}\right] + \tilde{T}_2\left[\frac{Z_1e^2}{\hbar v}\right]^2 + \cdots , \tag{29}$$

where the coefficients depend only on $\hbar\omega/2mv^2$. We also introduce the notation

$$\Delta E_B = \left[\frac{Z_1e^2}{\hbar v}\right]^2 \hbar\omega\tilde{T}_B \tag{30}$$

for the Barkas-effect, i.e., the difference in energy transfer for positive and negative particles.

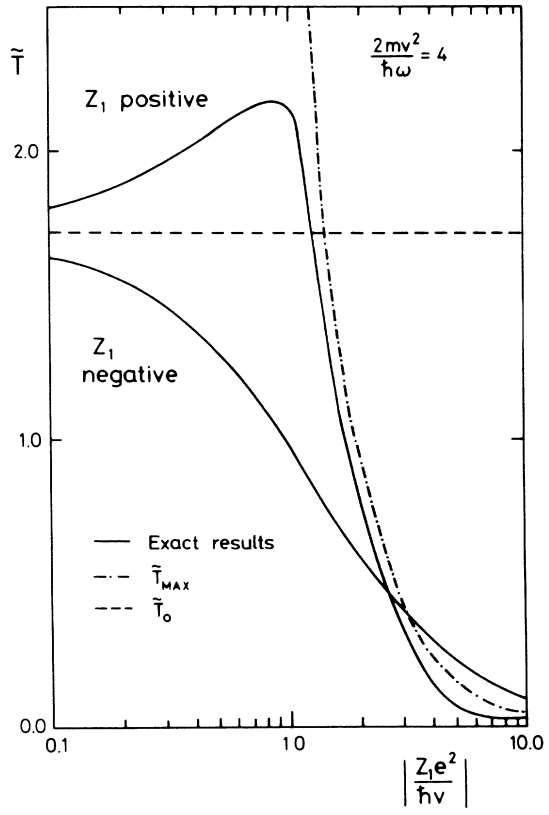

FIG. 1. The mean energy transfer in a central collision vs $|Z_1e^2/\hbar v|$ for the binding parameter $2mv^2/\hbar\omega=4$. Solid line, exact numerical results; dot-dashed line, maximum energy transferrable to a free electron at rest; dashed line, first Born approximation (Ref. 14).

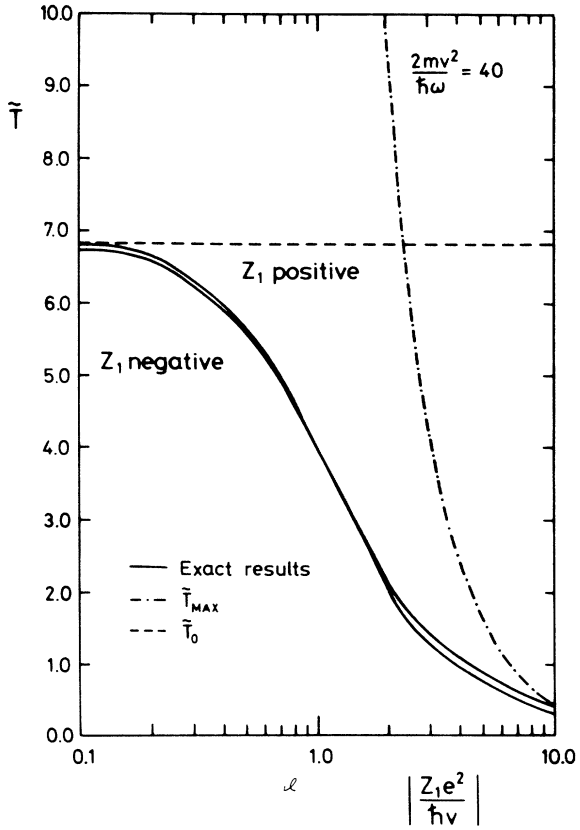

FIG. 2. The same as Fig. 1 for $2mv^2/\hbar\omega=40$.

We have computed numerically exact results for $\tilde{T}$ in the region $0.1 \le Z_1e^2/\hbar v \le 10.0$ and $1.0 \le 2mv^2/\hbar\omega \le 40.0$, and the Born coefficients $\tilde{T}_n$ for $n=0,1,\ldots,8$ and $1.0 \le 2mv^2/\hbar\omega \le 40.0$. The results for $\tilde{T}_0$, $\tilde{T}_1$, and $\tilde{T}_2$ have been compared with the corresponding results in Refs. 11, 14, and 15, and agreement within 1% was found.

In Figs. 1 and 2 we investigate the general dependence of $\tilde{T}$ on $Z_1e^2/\hbar v$ for two values of $\hbar\omega/2mv^2$ corresponding to relatively strong binding ($2mv^2/\hbar\omega=4$) and relatively weak binding ($2mv^2/\hbar\omega=40$) at identical velocities. For comparison, we have included $\tilde{T}_0$ based on the first Born approximation[14] and the maximum energy transferrable to a free electron at rest $\Delta E_{\max}=2mv^2$, which in the present notation yields

$$\tilde{T}_{\max} = \frac{2mv^2}{\hbar\omega}\left[\frac{\hbar v}{Z_1e^2}\right]^2 . \tag{31}$$

As expected, $\tilde{T}_0$ is approached for $|Z_1e^2/\hbar v| \ll 1$, where the interaction between the projectile and the bound electron is weak, while free-particle scattering prevails in the opposite limit $|Z_1e^2/\hbar v| \gg 1$. Turning to the Barkas correction, we see that the difference in energy transfer for positive and negative projectiles is quite large in the case of strong binding ($2mv^2/\hbar\omega=4$) leading to a pronounced maximum around $Z_1e^2/\hbar v \simeq 1$ for positive ions. In this region the energy transfer of a positive ion is

a factor of 2 larger than for the corresponding negative ion. In the case of weak binding ($2mv^2/\hbar\omega=40$) the difference is much smaller, although not quite negligible for large values of $Z_1e^2/\hbar v$. Such differences between the strong and weak binding limits are to be expected since the Barkas effect as a polarization effect must depend strongly on the magnitude of the binding force. In both cases the energy transfer is larger for positive projectiles than for negative ones in agreement with $\tilde{T}_1$, being positive in this region.[11] At larger values of $Z_1e^2/\hbar v$, however, the effect changes sign. This indicates that negative higher-order terms $\tilde{T}_{2n+1}$, $n>1$ are significant.

As the approach to $\tilde{T}_0$ in the limit $Z_1e^2/\hbar v \ll 1$ is quite different in the two cases considered, it is evident that the convergence behavior of the Born series must depend strongly on $\hbar\omega/2mv^2$. This is illustrated in Fig. 3, where we have plotted $\tilde{T}_n$ for $0\le n\le 8$. For $2mv^2/\hbar\omega=4$, the coefficients oscillate but fall off rapidly with $\tilde{T}_1$ being the dominating higher-order correction. However, for $2mv^2/\hbar\omega=40$ the picture is quite different. Both even and odd terms form alternating series, but while the even terms are all large, the first odd terms (notably $\tilde{T}_1$) are very small. The most important higher-order correction in this limit is therefore the negative fourth-order term $\tilde{T}_2$. Note that the sign and magnitude of the even terms for $2mv^2/\hbar\omega=40$ are consistent with the expansion of the Bloch correction for close collisions in (2). This is to be expected since the binding is of negligible importance when $\hbar\omega/2mv^2 \ll 1$.

In Figs. 4 and 5 we compare the Born series $\tilde{T}=\sum_{k=0}^{k_{\max}}\tilde{T}_k(Z_1e^2/\hbar v)^k$ for various values of $k_{\max}$ with the exact numerical results. As expected from Fig. 3, the convergence is more rapid in the case of strong binding ($2mv^2/\hbar\omega=4$), but in general we see that a series expansion is useful only for $Z_1e^2/hv<1$.

The condition $|Z_1e^2/\hbar v|<1$ puts a rather strong limit on the use of the Born approximation. This is illustrated in Figs. 6–8, where the dependence of ΔE on $2mv^2/\hbar\omega$ is plotted for positive and negative values of Z_1 at a fixed binding energy of $\hbar\omega=1$ Ry. We see that the first Born approximation is a reasonable starting point for $|Z_1|=1$ at high projectile energies. Even in this limit, however, the first Born approximation becomes inaccurate for $|Z_1|=2$ and 4. Furthermore, it is seen that while the Barkas correction is dominating for $|Z_1|=1$ negative, even corrections become increasingly important for heavier ions in agreement with the Bloch formula.

At low projectile energies ΔE approaches $\Delta E_{\max}=2mv^2$, i.e., the maximum energy transferrable to a free target electron at rest. The characteristic maximum of ΔE is thus a consequence of its different behavior in the low- and high-energy limits. Note, however,

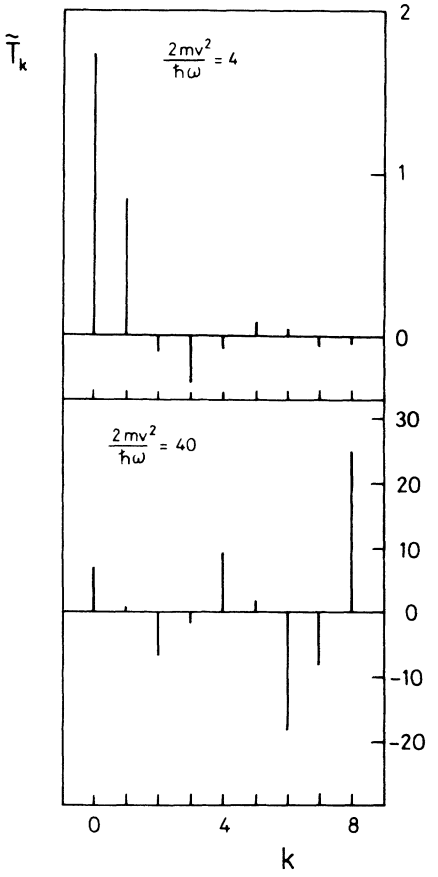

FIG. 3. The Born coefficients for the mean energy transfer in a central collision. $2mv^2/\hbar\omega=4$ and $2mv^2/\hbar\omega=40$.

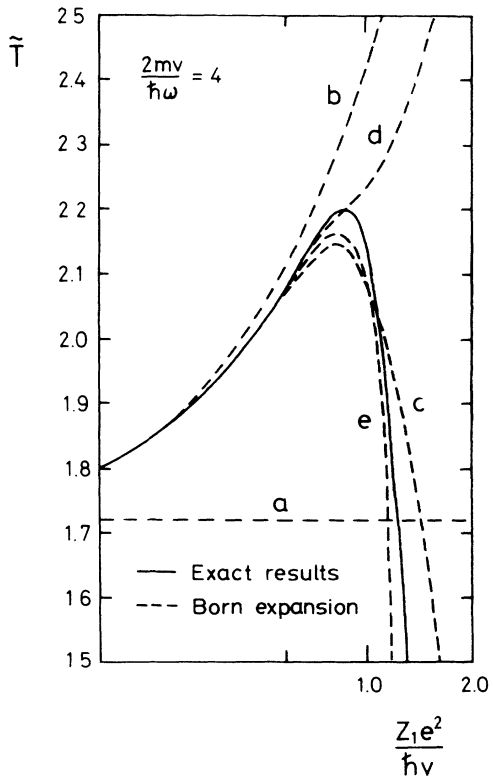

FIG. 4. Comparison of the Born expansion with exact numerical results for $2mv^2/\hbar\omega=4$. Solid line, exact numerical results; dashed line, the Born series $\tilde{T}=\sum_{k}^{k_{\max}}\tilde{T}_k(Z_1e^2/\hbar v)^k$ for $k_{\max}=0$, 2, 4, 6, and 8 corresponding to the curves a–e.

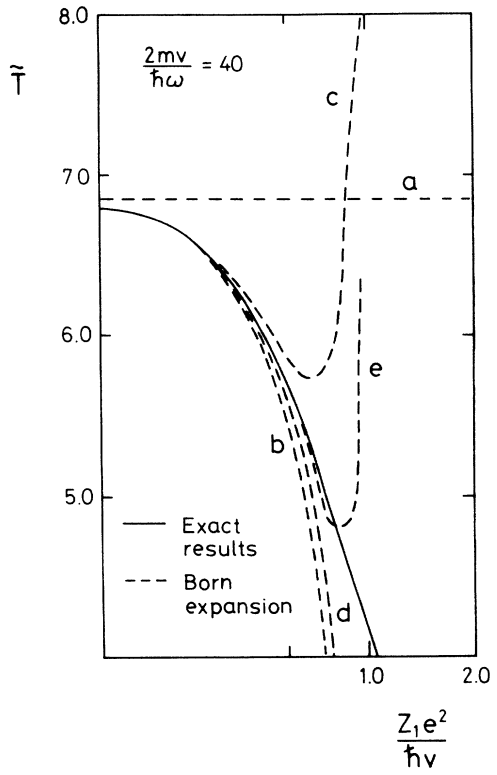

FIG. 5. The same as Fig. 4 for $2mv^2/\hbar\omega = 40$.

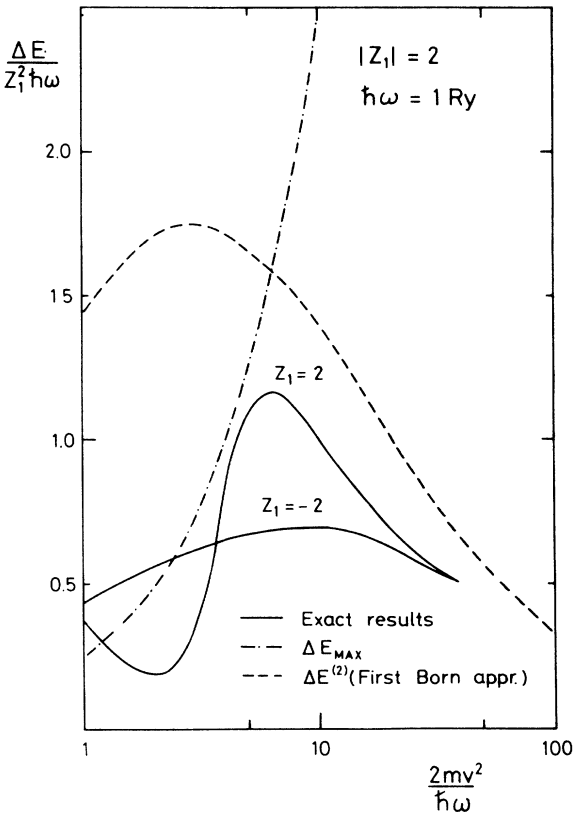

FIG. 7. The same as Fig. 6 for $|Z_1| = 2$.

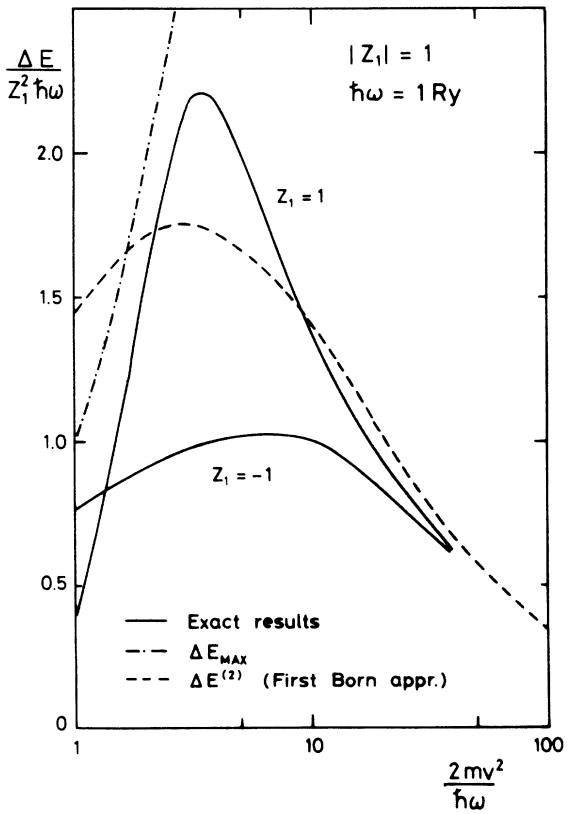

FIG. 6. Mean energy transfer vs projectile energy for $|Z_1| = 1$ and $\hbar\omega = 1$ Ry. Solid line, exact numerical results; dot-dashed line, maximum energy transferrable to a free electron at rest; dashed line, first Born approximation (Ref. 14).

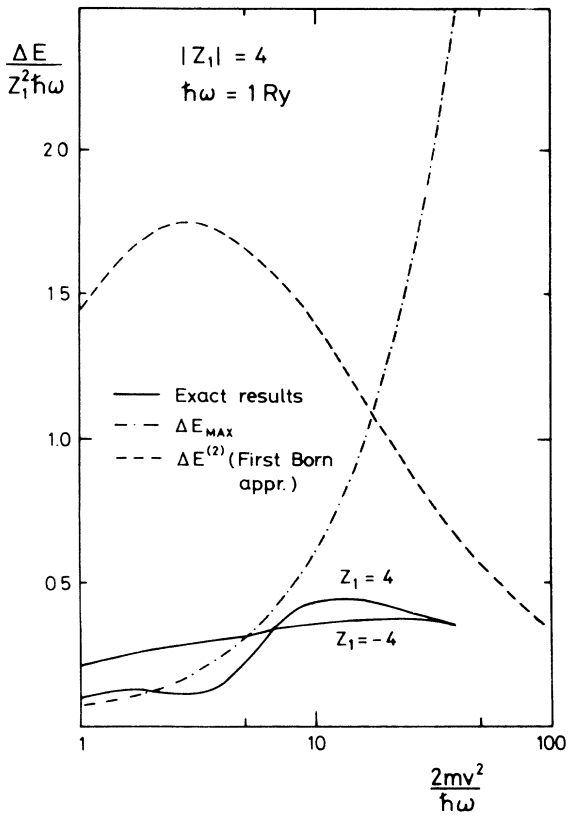

FIG. 8. The same as Fig. 6 for $|Z_1| = 4$.

that the overall behavior of ΔE depends critically on the sign of the interaction. For positive ions, the energy transfer is rather strongly peaked around the maximum value, while it is broad and featureless for negative ions. Some of the essential processes causing the strong energy dependence of ΔE in an attractive potential, where the projectile and the electron may come very close, are therefore suppressed in a repulsive potential.

In Fig. 9 we have plotted ΔE_B for the same values of $|Z_1|$ as in Figs. 6–8. As expected, large deviations from the perturbative result occur for low projectile energies, where the binding is important. In the high-energy region, however, the perturbative result is approached and the Barkas correction becomes quite small even for heavy ions. This indicates that while the overall applicability of the Born series is determined by $Z_1e^2/\hbar v$, the odd terms show an additional strong velocity dependence due to the binding parameter $\hbar\omega/2mv^2$.

V. DISCUSSION

We have calculated the mean energy transferred to a quantum harmonic oscillator in a central collision with a uniformly moving point charge. The calculation was carried out numerically by solving the time-dependent Schrödinger equation in a basis of energy eigenfunctions of the undisturbed oscillator. The energy transfer ΔE is given numerically exact and up to tenth order in a Born series.

As expected from Ref. 4, we find a clear separation of the results according to the value of $Z_1e^2/\hbar v$. For $|Z_1e^2/\hbar v| \ll 1$ the interaction between the projectile and the electron is weak and causes only a small disturbance of the motion of the bound electron. In the opposite limit of $|Z_1e^2/\hbar v| \gg 1$ the interaction is strong, and in this case the binding causes a small correction in an otherwise free collision. A Born series in $Z_1e^2/\hbar v$ is therefore useful only for light ions, while a more-detailed treatment is needed for heavier ions, where the two regions must be connected. The numerical method developed in this paper provides an example of such an approach.

Our results confirm that a Barkas correction exist even in the case of a central collision, where the interaction time is short compared to that of a distant collision. The Barkas correction, however, turns out to depend strongly on the binding parameter $\hbar\omega/2mv^2$. At low velocities it is a very large correction, but at higher velocities it vanishes even for heavier ions, while large, even corrections persist in this limit.

In a more general context, the results of the present calculation of ΔE for a central collision support the inclusion of a Bloch correction for close collisions. However, in the presence of a binding force a close-collision Barkas correction must also be considered. Only when $\hbar\omega/2mv^2 \ll 1$ does the Barkas correction become very small and an expansion in even terms of $Z_1e^2/\hbar v$ is possible.

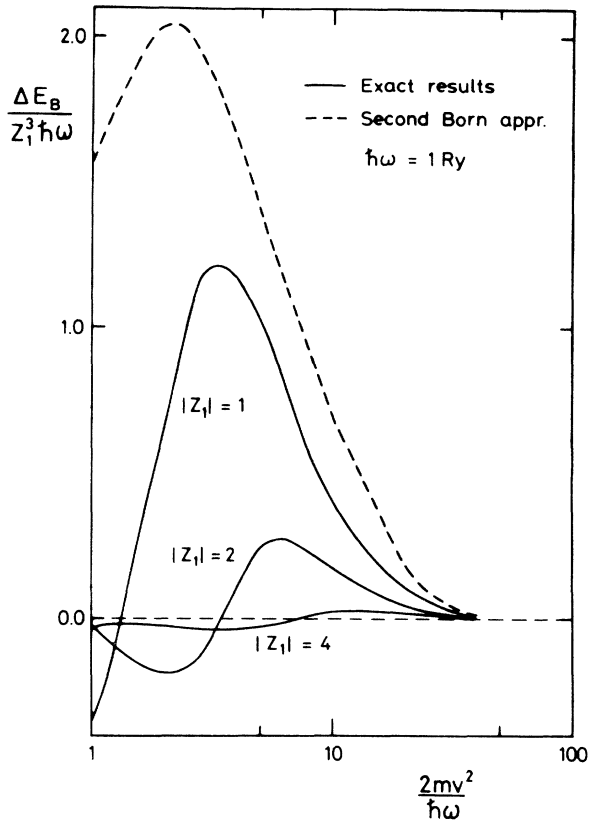

FIG. 9. The Barkas correction vs projectile energy for $|Z_1|=1$, $|Z_1|=2$, and $|Z_1|=4$. In all cases $\hbar\omega=1$ Ry. Solid line, exact numerical result; dashed line, Barkas correction based on the second Born approximation (Ref. 11).

As the methods of calculation presented here are quite general, they are applicable to more realistic atomic potentials also. This is important since quantitative aspects of the calculation may depend on the particular choice of binding force. Considering, however, the harmonic oscillator as a limiting case of a general atomic system characterized by a mean resonance frequency $I/\hbar$,[19] we may assume that the qualitative features of the calculation are general.

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