Matrix analysis of classical elastic collisions

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The velocities of two bodies before and after an elastic collision can be related by a matrix transformation in one and two dimensions. We demonstrate a very simple relation between the one- and two-dimensional collision matrices. © *2007 American Association of Physics Teachers.*
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I. INTRODUCTION

The standard texts in classical mechanics[1-3] treat binary collisions in the center of mass frame and then discuss scattering by a central force without offering a method for dealing with collisions in arbitrary inertial frames. This note presents a technique for handling such cases in two dimensions using complex scattering matrices. The technique has several applications in the classroom including how complex numbers can be useful in classical mechanics, a field where the use of complex numbers is rare. The method also gives a classical context to certain ideas that are more commonly associated with quantum mechanics, such as state vectors and operators, thus allowing these topics to be introduced earlier in the curriculum. Finally, the method can be used in mathematical physics classes to provide an illustration of matrix exponentiation with a real power, in which the matrix and exponent each have a clear physical meaning.

When a particle of mass m and velocity u and a particle of mass M and velocity v collide elastically in one dimension, their velocities after the collision, u' and v', respectively, are uniquely determined by u and v. The reason is that u' and v' are determined from the conservation equations for energy and linear momentum. These equations are

$$mu + Mv = mu' + Mv', \tag{1}$$

$$\tfrac{1}{2}mu^2 + \tfrac{1}{2}Mv^2 = \tfrac{1}{2}mu'^2 + \tfrac{1}{2}Mv'^2, \tag{2}$$

and are readily solved. If we ignore the trivial nonscattering solution, $u'=u$ and $v'=v$, the final velocities may be expressed in terms of the initial ones and the appropriate scattering matrix S_1 as

$$\begin{pmatrix} u' \\ v' \end{pmatrix} = S_1 \begin{pmatrix} u \\ v \end{pmatrix} = \frac{1}{m+M}\begin{pmatrix} m-M & 2M \\ 2m & M-m \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}. \tag{3}$$

In two dimensions, where there are four unknown velocity components, two for each particle, but only three conservation equations (one for energy and two for linear momentum), there is one remaining degree of freedom in the solution. This degree of freedom may be interpreted as the scattering angle, α, of the collision in the center of mass frame. The natural scattering matrix would be a 4×4 matrix function of α. However, if we represent the particle velocities by complex numbers, we can find a 2×2 complex matrix, S_2, which transforms the precollision velocities to the postcollision velocities. We now further analyze the one-dimensional case and demonstrate the relation between S_1 and S_2. The eigenvalues of S_1 are 1 and -1 with normalized eigenvectors:

$$\mathbf{e}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{4a}$$

$$\mathbf{e}_- = \frac{1}{\sqrt{m^2+M^2}}\begin{pmatrix} M \\ -m \end{pmatrix}, \tag{4b}$$

respectively. The matrix can be written in standard spectrally decomposed form as

$$S_1 = (+1)P_{+1} + (-1)P_{-1}, \tag{5}$$

where

$$P_{+1} = \frac{1}{(m+M)}\begin{pmatrix} m & M \\ m & M \end{pmatrix}, \tag{6a}$$

$$P_{-1} = \frac{1}{(m+M)}\begin{pmatrix} M & -M \\ -m & m \end{pmatrix} \tag{6b}$$

are the projection operators onto the eigenvectors $\mathbf{e}_+$ and $\mathbf{e}_-$, respectively. The coefficient of -1 in Eq. (5) serves to flip the velocities in the center of mass frame.

Equation (5) may be interpreted as follows. The projector P_{+1} extracts the velocity of the center of mass frame, that is,

$$P_{+1}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} w_{\mathrm{cm}} \\ w_{\mathrm{cm}} \end{pmatrix}, \tag{7}$$

where w_{cm} is the velocity of the center of mass frame. Because w_{cm} is unchanged in the collision, this projector has a coefficient of $+1$. The projector P_{-1} extracts the velocities as they appear in the center of mass frame, that is,

$$P_{-1}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u - w_{\mathrm{cm}} \\ v - w_{\mathrm{cm}} \end{pmatrix}. \tag{8}$$

In the center of mass frame, the effect of the collision is to flip the signs of the velocities; this is handled by the coefficient of -1 in front of P_{-1}.

We now consider the two-dimensional case and modify Eq. (5) to obtain the equation for S_2. In two dimensions, as in one, the total momentum of the particles in the center of mass frame is zero, before and after the collision. This fact, together with conservation of energy, implies that the collision may only rotate the velocities through an angle, which is

The Runge–Lenz vector for the two-dimensional hydrogen atom

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The recent discovery of novel properties possessed by two-dimensional systems has led to the investigation of properties of the hydrogen atom in two dimensions. With proper definition of the system, the so-called Runge–Lenz vector may be defined for this system, and shown to be related to the underlying $O(3)$ symmetry, just as for the three-dimensional system, although some interesting aspects are revealed.

I. INTRODUCTION

Much interest has been developing in the properties of two-dimensional systems. The existence of Chern–Simons terms[1] and the existence of anyons[2] that violate the theorem on spin and statistics are but two examples. There are also examples where two-dimensional behavior has been exhibited experimentally, such as the propagation of electrons in high-T_c superconductors, where the two-dimensionality is apparently imposed by the planes of copper atoms.[3] For the latter systems in particular the analysis of the two-dimensional hydrogen atom may be particularly relevant.

It is by now well known that the hydrogen atom in three dimensions exhibits an "accidental degeneracy" due to a "hidden" four-dimensional rotational group [$O(4)$] symmetry and the presence of an additional conserved vector, most commonly called the Runge–Lenz vector although actually much older than these two authors.[4] Indeed, in 1935 Fock[5] showed how to cast the momentum-space form of the Schrödinger integral equation into the equation for $O(4)$ hyperspherical harmonics. The connection of this approach with the older Runge–Lenz vector approach utilized by Pauli[6] in his solution of the hydrogen atom problem was exhibited by Bargmann,[7] who showed that linear combinations of the components of the Runge–Lenz vector and the angular momentum vector obeyed the commutation relations of the Lie algebra of $O(4)$ [or, more precisely, of $O(3)\times O(3)$ which is isomorphic to $O(4)$].

The approach of Fock was generalized to d dimensions by Alliluev.[8] In particular, he showed that the hydrogen atom in d dimensions exhibits the symmetry of the $(d+1)$-dimensional rotation group when expressed in momentum space, and the wave functions are nothing more than hyperspherical harmonics. His solution also pertains for the case $d=2$. In this case he finds for the energy levels in atomic units:[9]

$$E_n = -1/2(n-\tfrac{1}{2})^2, \tag{1}$$

where $n = 1,2,3,\ldots$, and the momentum space wave functions are the ordinary $O(3)$ spherical harmonics Y_{nm}. However, the analogous $d=2$ generalization of the Runge–Lenz vector does not appear to have been previously discussed, so that is the gap that we feel it is now opportune to fill.

Before turning to the main body of this work, it is perhaps worth mentioning that there is some controversy as to the "correct" generalization of the Coulomb potential. Our approach is based on a potential proportional $1/r$, where r is the distance from the origin in d-dimensional space. An alternative definition, which coincides in the case $d=3$, arises from the desire to preserve Maxwell's equations, and particularly Gauss' law: The electric flux through a spherical hypersurface should be proportional only to the total charge enclosed, and be independent of the radius of the sphere. For $d=2$ this gives rise to a potential proportional to $\ln(r)$. For a recent paper on this potential see Ref. 10. However, it is our view that the $1/r$ potential is the more natural for $d=2$ since there are cases in which the motion of the electron around the nucleus is constrained in a plane by certain boundary conditions. The planar confinement to such a system can be a result of extreme anisotropy.

II. THE 2-D HYDROGEN ATOM

In two dimensions the Hamiltonian of our system may be written (using atomic units):

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) - 1/r. \tag{2}$$

The angular momentum vector degenerates to a single component $L = L_z$:

$$L = xp_y - yp_x. \tag{3}$$

The Runge–Lenz vector $\mathbf{A}$, which in three dimensions is defined by

$$\mathbf{A} = \mathbf{r}/r - \tfrac{1}{2}(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}), \tag{4}$$

degenerates to a two-dimensional vector:

$$A_x = x/r - \tfrac{1}{2}(p_yL + Lp_y),$$
$$A_y = y/r + \tfrac{1}{2}(p_xL + Lp_x). \tag{5}$$

The three quantities L, A_x, and A_y all commute with H and so are conserved. Their mutual commutation relations can be shown to be

$$[L, A_x] = iA_y, \tag{6}$$

$$[L, A_y] = -iA_x, \tag{7}$$

and

$$[A_x, A_y] = -2iHL. \tag{8}$$

Now, let us assume that the operators are operating on states that are all eigenstates of H with eigenvalue E, which we take to be negative, since we are interested in bound states. If we define new operators on this manifold:

$$\mathbf{u} = \mathbf{A}/\sqrt{(-2E)}, \tag{9}$$

then we may define a *three*-dimensional vector operator $\mathbf{N}$, with components $N_x = u_x$, $N_y = u_y$, and $N_z = L$ that satisfy the commutation relations characteristic of the components of an ordinary angular momentum operator in three dimensions. That is, using $H \to E$ in Eq. (8):

$$[N_i, N_j] = i\epsilon_{ijk}N_k. \tag{10}$$

These define the Lie algebra su(2), and familiar arguments

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Retardation in two-photon absorption

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Previous calculations of two-photon absorption and emission in hydrogen have revealed frequencies at which the transition is forbidden, at least within the approximations made. Here we show that if retardation is taken into account these so-called "transparency frequencies" are slightly shifted, but the zero transition amplitude persists.

INTRODUCTION

In recent papers on two-photon absorption and emission processes in atomic hydrogen,[1] it was discovered that certain photon frequencies were forbidden. Considering emission, for example, in the $3s$- $1s$ transition, there are two photons emitted of frequencies ω_A and ω_B such that the total energy of the two photons equals the energy difference between the $3s$ and $1s$ levels, i.e., 12 eV. However, the amplitude for this process passes through two zeros, symmetrically placed on either side of the equal frequency point $\omega_A=\omega_B$. (There are no zeros in the two-photon decay of the $2s$ metastable state.) The same amplitude governs the two-photon absorption process $1s$-$3s$, and so there exist two frequencies at which this absorption cannot take place; we call these the "transparency frequencies"[2] for either emission or absorption. Thus, since there is no corresponding amplitude zero at these transparency frequencies for the $1s$-$3d$ process, there is suggested a means for selective excitation of the $3d$ level. Transparency frequencies were found[1] for transitions between the $1s$ and ns levels for $n=3$, 4, 5, and 6, between the $1s$ and nd levels for $n=4$, 5, and 6, between the $2s$ and ns levels for $n=4$, 5, and 6, and between the $2s$ and nd levels for $n=5$ and 6.

The above remarks are based on calculations which use second-order perturbation theory and the dipole (long-wavelength) approximation.[1] It has recently been suggested to the authors[3] that the transparency phenomenon might disappear when retardation effects are taken into account. The reason for this expectation is that the amplitude as previously calculated is the sum of two terms, each representing one ordering of the emission of the two photons. In the dipole approximation these two terms are *real* for the $1s$-$3s$ case, and at the transparency frequencies they exactly cancel (in other cases the two terms are sometimes purely imaginary, with the same result). However, when retardation is included the relevant matrix elements would appear to be complex, and the cancellation thus much more unlikely. The purpose of this Brief Report is to show that simple parity arguments indicate that the terms remain real (or pure imaginary if the conventions of Ref. 1 are followed), but shift their value slightly. Thus the transparency condition persists, albeit at slightly shifted frequencies.

CALCULATION

When retardation is taken into account, the ns-$1s$ transition rate is proportional to the square of the modulus of the second-order perturbation theory expression

$$A_{ns\text{-}1s} \propto \left| \sum_I \left[\frac{M_I^{(1)}}{E_I\text{-}E_1\text{-}h\omega_B} + \frac{M_I^{(2)}}{E_I\text{-}E_1\text{-}h\omega_A} \right] \right|^2 , \quad (1)$$

where $M_I^{(1)}$ is

$$M_I^{(1)} = \langle ns | e^{i\mathbf{k}_A\cdot\mathbf{r}} \hat{\epsilon}_A\cdot\mathbf{p} | I \rangle \langle I | e^{i\mathbf{k}_B\cdot\mathbf{r}} \hat{\epsilon}_B\cdot\mathbf{p} | 1s \rangle , \quad (2)$$

and where I represents an arbitrary intermediate hydrogenic state including the continuum. In this expression $\hat{\epsilon}_A$ and $\hat{\epsilon}_B$ are the polarization vectors of the two photons. We have used the Coulomb gauge interaction Hamiltonian $-e\,\mathbf{A}\cdot\mathbf{p}/mc$, dropping the A^2 term which can never contribute to processes in which the electron changes energy levels. We note that this Hamiltonian differs from the $\mathbf{r}\cdot\mathbf{E}$ form used in our previous work[1] because the latter is equivalent to the $\mathbf{A}\cdot\mathbf{p}$ form only in the dipole approximation, whereas the $\mathbf{A}\cdot\mathbf{p}$ form is generally valid to all orders, according to the principle of minimal coupling. $M_I^{(2)}$ in Eq. (1) is the same as $M_I^{(1)}$ in Eq. (2) except for the exchange of the two photons, $A \leftrightarrow B$. Let us look at a typical matrix element of the form occurring in the M_I:

$$\langle nlm | e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\epsilon}\cdot\mathbf{p} | n'l'm' \rangle . \quad (3)$$

Using De Moivre's theorem we may write the operator

Third-Born-approximation effects in electron capture

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We have calculated corrections to the strong-potential Born approximation using the distorted-wave Born formalism of Taulbjerg and Briggs. In the sense of a plane-wave Born expansion, all terms of the third Born approximation, and all "single switching" fourth Born terms are included, but a peaking approximation is needed to reduce the calculation to tractable form. We believe this to be the first calculation to be so complete in the Born sense. Effects of the higher terms are most visible in the valley between the Thomas peak and the forward peak. The Thomas peak is visible in the correction term even though it includes no second Born contributions. We suggest that this may be interpreted as a third Born effect with two "hard" collisions followed by a "soft" collision.

INTRODUCTION

The experimental observation of the Thomas peak in electron capture by energetic ions[1-3] has given new credibility to our theoretical understanding of the capture process. In particular, the development of the so-called strong-potential Born (SPB) approximation,[4-11] which is in reality a kind of distorted-wave first Born approximation, has given new confidence in the ability of theory to account for some of the more subtle features of the capture process.

In this paper we report the results of an attempt to go beyond the SPB. Just as the SPB approximation, if expanded in a plane-wave Born series can be said to include all second Born contributions, plus higher contributions in one of the potentials (designated the "strong" potential), the expression we use includes all the third Born contributions and all but one of the fourth Born terms, as well as higher terms. We cannot evaluate these additional terms exactly, but as a small correction to the SPB cross section, we felt justified in evaluating them using a "peaking approximation." The results show that the correction is indeed small, but surprisingly, at very high energies it shows a Thomas peak effect, and a significant contribution exceeding the SPB in the region of the "valley" between the forward and the Thomas peaks.

THEORY

Our starting point is the expression due to Taulbjerg and Briggs,[12] which they call the distorted-wave Born (DWB) approximation:

$$T_{fi}^{\mathrm{DWB}}=\langle\chi_f^-\mid V_P\mid\chi_i^+\rangle-\langle\Phi_f\mid V_P\mid\chi_i^+-\Phi_i\rangle\ . \tag{1}$$

The distorted waves are

$$\mid\chi_i^+\rangle=(1+G_P^+V_P)\mid\Phi_i\rangle\ , \tag{2a}$$

$$\mid\chi_f^-\rangle=(1+G_T^-V_T)\mid\Phi_f\rangle\ , \tag{2b}$$

with asymptotic wave functions

$$\Phi_i(\mathbf{r}_T,\mathbf{R}_T)=\frac{e^{i\mathbf{K}_i\cdot\mathbf{R}_T}}{(2\pi)^{3/2}}\phi_i(\mathbf{r}_T)\ , \tag{3a}$$

$$\Phi_f(\mathbf{r}_P,\mathbf{R}_P)=\frac{e^{i\mathbf{K}_f\cdot\mathbf{R}_P}}{(2\pi)^{3/2}}\phi_f(\mathbf{r}_P)\ , \tag{3b}$$

which describe the initial and final particle states, respectively. By inserting the expressions (2) in Eq. (1), the DWB matrix element can be written

$$T_{fi}^{\mathrm{DWB}}=\langle\Phi_f\mid(1+V_TG_T^+)V_P\mid\Phi_i\rangle+\langle\Phi_f\mid V_TG_T^+V_PG_P^+V_P\mid\Phi_i\rangle\ . \tag{4}$$

The first term can be recognized as the SPB amplitude, so that the second term represents the DWB correction. While this expression appears to be asymmetric in its treatment of the potentials V_P and V_T, Taulbjerg and Briggs[12] show that it is nevertheless symmetric. They also show by an expansion of the Green's functions G_P^+ and G_T^+ in terms of the plane-wave Green's function G_0^+ that the DWB expression includes all the third Born terms, i.e., $V_TG_0^+V_TG_0^+V_P$ and $V_TG_0^+V_PG_0^+V_P$, three of the four terms of the fourth Born approximation (all the "single switch" terms).

$$V_TG_0^+V_TG_0^+V_TG_0^+V_P\ ,$$

$$V_TG_0^+V_PG_0^+V_PG_0^+V_P\ ,$$

and

$$V_TG_0^+V_TG_0^+V_PG_0^+V_P$$

are included while the "triple switch" term $V_TG_0^+V_PG_0^+V_TG_0^+V_P$ is missing.

We evaluated the first (SPB) term of Eq. (4) using the techniques of Sil and McGuire[8] (see Table I). For the second (DWB) term we use manipulations similar to those of Macek and Alston[6] to reduce the expression to the form

Strong-potential Born-approximation calculations of $1s$-$2p$ electron capture

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Cross sections for electron capture into the $2p$ level evaluated with use of the strong potential Born approximation are presented. While these $2p$ cross sections are smaller than cross sections for capture into the $1s$ and $2s$ levels at high velocities, nevertheless the Thomas peak is clearly evident at energies above 1 MeV in both the $m=0$ and $|m|=1$ magnetic substates in atomic hydrogen. At energies above 10 MeV where the Thomas peak is important, cross sections for capture into $m=0$ and $|m|=1$ are comparable. Consequently, the polarization fraction becomes negative at high energies in sharp contrast to Brinkman-Kramers results where the polarization fraction stays near its maximum value.

I. INTRODUCTION

Considerable progress has been achieved in understanding electron capture at high velocities in terms of a two-step mechanism for $1s$-$1s$ capture. On the one hand the qualitative nature of this mechanism may be understood in terms of the simple classical two-step model introduced[1] by Thomas in 1927. On the other hand quantitative understanding has also been achieved with the development of quantal calculations which include second-order effects. Of these quantal calculations perhaps the most successful has been[2-7] the SPB, or strong-potential Born approximation. In the SPB approximation the intermediate states of the collision system are represented by continuum states in the stronger, target or projectile, Coulomb fields. A definitive confirmation of this picture has been provided by observation[8] of the Thomas peak in the differential cross section.

While understanding of the $1s$-$1s$ cross section dominant for capture at high velocities seems well in hand, the $1s$-$2p$ cross section is not so well understood. For example, the full peaking (FP) approximation, SPB-FP, which is apparently quite satisfactory[2,9,10] for $1s$-ns capture in charge asymmetric systems, gives zero cross sections for $1s$-$2p$ capture. Furthermore, the continuum distorted wave (CDW) approximation,[11-13] which gives satisfactory results for $1s$-$1s$ capture, does not reproduce the correct second Born limit for $1s$-$2p$ capture. Moreover, Briggs and Dubé[14] have emphasized that striking differences are generally expected between first- and second-order theories for large n and l at high velocities. Hence, new understanding may be obtained from studies of $1s$-nl capture.

In this paper we present expressions for $1s$-np capture in the SPB approximation. We use the technique[7] of Sil and McGuire (SM) which avoids the peaking approximation in the Green's function that results in zero $1s$-np SPB cross sections. Furthermore, it has been demonstrated[15] that the SM technique may be applied to systems of arbitrary target and projectile charges, i.e., ignoring a weaker potential is not necessary using the SM technique. The SM $1s$-np expressions are presented in Sec. II. Results of calculations for $1s$-$2p$ capture in $p+\mathrm{H}$ are presented and discussed in Sec. II.

II. THEORY

In this section we present SPB amplitudes for $1s$-np electron capture using the technique[7] of Sil and McGuire. Atomic units are used and we follow the notation of SM.

First, we express the three np wave functions in momentum space, $\tilde{\phi}_{np}^{+1}$, $\tilde{\phi}_{np}^{0}$, and $\tilde{\phi}_{np}^{-1}$, as follows:

$$\tilde{\phi}_{np}^{+1}=\frac{-\sqrt{2}\Phi p_0}{\sqrt{\pi}(p^2+p_0^2)}(p_x+ip_y)\,, \tag{1}$$

$$\tilde{\phi}_{np}^{0}=\frac{2\Phi p_0}{\sqrt{\pi}(p_0^2+p^2)}p_z\,, \tag{2}$$

$$\tilde{\phi}_{np}^{-1}=(\tilde{\phi}_{np}^{+1})^*\,, \tag{3}$$

where

$$\Phi=\left[\frac{32}{\pi}\right]^{1/2}\frac{p_0^{5/2}}{(p^2+p_0^2)^2},\quad p_0=\frac{Z_p}{n}\,, \tag{4}$$

and

$$\begin{aligned} p_x&=p\sin\theta\cos\phi\,,\\ p_y&=p\sin\theta\sin\phi\,,\\ p_z&=p\cos\theta\,. \end{aligned} \tag{5}$$

The starting point to evaluate capture amplitude is (3.12) of SM, which is

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Are Quantum Waves Observable?

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Summary. — An experiment has been proposed to test whether an objective physical reality can be granted to probability amplitudes. We consider an idealized version of the experiment and show that quantum mechanics predicts a null result.

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1. – Introduction.

The probability amplitude represents perhaps the most striking departure of quantum theory from classical physics. This is seen convincingly in the two-slit experiment, which in a sense « contains the *only* mystery » of quantum mechanics (1). The two-slit experiment shows how the concept of a probability amplitude resolves the paradox of wave-particle duality.

In what sense, if any, can an objective physical reality be attached to the probability amplitude? This question has recently been raised by SELLERI (2),

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Influence of the linear Stark effect on electron exchange in the eikonal calculations

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The eikonal approximation taking into account the post-collisional Stark effect removes the shortcoming of the previous calculations of relative l capture cross sections. We find good agreement between the calculated σ_{2s} and σ_{2p} cross sections and the available experimental data in $p+\mathrm{H}(1s)$ collisions.

In a series of papers[1-6] an eikonal approach[7,8] to electron capture from $\mathrm{H}(1s)$ into fast multichanged projectile ions has been proposed. The results obtained are not only in better agreement with experimental findings for hydrogen and helium targets, but have a remarkable simplicity, comparable with that of the simplest first-order theory, the Oppenheimer-Brinkmann-Kramers (OBK) approximation. However, the successes of the eikonal approximation reported so far have been *only partial,* since there is an overestimate of the $l \neq 0$ cross section compared with the corresponding s cross section for the same principal shell.

In a recent interesting publication[9] Burgdörfer pointed out the importance of the Stark mixing between the degenerate excited states of the projectile escaping the field of the residual target ion and named the coupling between states of the same principal shell long after the primary charge transfer has taken place the "post-collision interaction" (PCI). Applying the PCI model to the OBK approximation for the primary capture processes, Burgdörfer found improved agreement of the relative l cross section and the alignment parameter with experimental data. The agreement only holds for *relative, but not for the absolute* substate cross sections. In this paper, we apply the PCI model together with the eikonal approximation to study the σ_{2s} and σ_{2p} capture cross sections in $p+\mathrm{H}(1s)$ collisions. Atomic units are used throughout.

Consider the capture of an electron initially bound in the $1s$ shell of a hydrogenic target with charge Z_t into a given n,l,m state of a bare projectile ion with charge Z_p. In the eikonal approach the transition amplitude can be written as[5]

$$A_{1s-nlm}(\vec{b}) = \frac{i2\pi Z_p}{v}\int d^2p_b\,[g^*_{nlm}(\vec{p}+\vec{v})\,G_{1s}(\vec{p})]_{p_z=p_{0z}}\,e^{-i\vec{b}\cdot\vec{p}_b}\ , \tag{1}$$

where $p_{0z} = -\frac{1}{2}v+\eta\epsilon$ with $\eta = 1/v$ and the energy defect $\epsilon = -Z_p^2/2n^2 + Z_t^2/2$. In Eq. (1), g_{nlm} and G_{nlm} are defined and given by Eqs. (14) and (21), respectively, in Ref. 5. The phase factor[10] $(-i)^l$ in g_{nlm}, which was dropped in Ref. 5, is very important and must be retained in the present study.

Following Burgdörfer,[9] the eikonal amplitudes within the PCI model are related to the usual eikonal amplitudes [Eq. (1)] by an evolution operator, namely,

$$A^{\mathrm{PCI}}_{2s}(\vec{b}) = \cos\phi A_{2s}(\vec{b}) + i\sin\phi A_{2p0}(\vec{b})\ , \tag{2a}$$

$$A^{\mathrm{PCI}}_{2p0}(\vec{b}) = \cos\phi A_{2p0}(\vec{b}) + i\sin\phi A_{2s}(\vec{b})\ , \tag{2b}$$

$$A^{\mathrm{PCI}}_{2p,\pm1}(\vec{b}) = A_{2p,\pm1}(\vec{b}) \tag{2c}$$

TABLE I. Calculated charge capture cross sections σ_{1s-2lm} (in 10^{-16} cm^2) for the reactions $\mathrm{H}^+ + \mathrm{H}(1s) \rightarrow \mathrm{H}(2lm) + \mathrm{H}^+$ as a function of energy. The results for eikonal both with and without the PCI model are tabulated. 5.088(−1) is an abbreviation for 5.088×10^{-1}.

Cross section (10^{-16} cm^2) \ Incident energy (keV)		30	50	70	100	150	200	500
Eikonal	σ_{2p}	5.088(−1)	1.331(−1)	4.268(−2)	1.034(−2)	1.617(−3)	3.771(−4)	2.022(−6)
	σ_{2s}	2.822(−1)	9.546(−2)	3.910(−2)	1.279(−2)	2.903(−3)	8.915(−4)	1.180(−5)
	$\frac{\sigma_{2p}}{\sigma_{2s}}$	1.803	1.394	1.092	0.808	0.557	0.423	0.171
Eikonal with PCI	σ_{2p}	2.013(−1)	6.183(−2)	2.106(−2)	5.309(−3)	8.527(−4)	2.012(−4)	1.099(−6)
	σ_{2s}	5.893(−1)	1.667(−1)	6.073(−2)	1.783(−2)	3.667(−2)	1.067(−3)	1.272(−5)
	$\frac{\sigma_{2p}}{\sigma_{2s}}$	0.341	0.371	0.347	0.298	0.233	0.189	0.087

Simple example in second-order perturbation theory

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A common problem faced by teachers of quantum mechanics is to find a good example to illustrate perturbation theory in the second order. Probably the most popular example is that of the quadratic Stark effect in hydrogen or, what is essentially the same thing, the (static) dipole polarizability of hydrogen. In the former case, to be definite, the hydrogen atom is perturbed by a uniform external field $\mathscr{E} = \mathscr{E}\hat{z}$. The perturbation term in the Hamiltonian is

$$H' = -e\mathscr{E}z. \tag{1}$$

The Stark shift in the ground state energy is then given by second-order perturbation theory as

$$E_1 = E_1^0 + e^2\mathscr{E}^2 \sum_{\substack{n\neq 1 \\ l,m}} \frac{|\langle 1,0,0|z|n,l,m\rangle|^2}{E_1^0 - E_n^0}, \tag{2}$$

where $|nlm\rangle$ is the unperturbed hydrogen state vector and E_n^0 the corresponding energy. The sum in Eq. (2) runs over the infinity of intermediate states other than the ground state, including the continuum, and its evaluation thus presents formidable problems for classroom presentation. One method requires the introduction of parabolic coordinates.[1] A simpler method was recently published in this journal.[2] Probably the simplest published treatment is that in the final edition of Schiff's textbook,[3] which is a version of the powerful but not well-known method of Dalgarno and Lewis,[4–6] which converts the infinite sum in Eq. (2) to a differential equation. Schiff integrates the differential equation by an expansion in power series, which he shows terminates after a few terms. The teacher can, of course, just produce this solution *ex nihilo*, but we have discovered what we believe to be a better alternative, which avoids solving the equation at all.

We begin by deriving the necessary differential equation. In the summation in Eq. (2), only the $l = 1$, $m = 0$ intermediate states contribute nonvanishing matrix elements, in accordance with the usual parity selection rules. If we write $z = r\cos\theta$ we can do the angular integral directly:

$$\int\int Y_{10}^*(\theta,\phi)\cos\theta Y_{00}(\theta,\phi)\sin\theta\, d\theta\, d\phi = \frac{1}{\sqrt{3}}, \tag{3}$$

where we have used the spherical harmonics

$$Y_{00}(\theta,\phi) = (4\pi)^{-1/2}$$

and

$$Y_{10}(\theta,\phi) = (3/4\pi)^{1/2}\cos\theta.$$

Thus,

$$\sum_{\substack{n\neq 1 \\ l,m}} \frac{|\langle 100|z|nlm\rangle|^2}{E_1^0 - E_n^0} = \frac{1}{3}\sum_{n\neq 1} \frac{|\langle R_{10}|r|R_{n1}\rangle|^2}{E_1^0 - E_n^0} = \frac{1}{3}\Sigma. \tag{4}$$

To calculate the sum Σ we define an auxiliary function $u(r)$ [which is $rf(r)$ in Schiff[2]]:

$$u(r) = \sum_{n\neq 1}\left[\left(rR_{n1}(r)\int_0^\infty R_{10}(r')R_{n1}(r')r'^3\, dr'\right) \times (E_1^0 - E_n^0)^{-1}\right], \tag{5}$$

where the $R_{nl}(r)$ are the radial factors of the hydrogen wave functions, satisfying, for $l = 1$ (we use units $m = \hbar = e = 1$):

$$\frac{1}{2}\frac{d^2}{dr^2}(rR_{n1}) + \left(\frac{1}{r} - \frac{1}{r^2}\right)(rR_{n1}) = -E_n^0(rR_{n1}) = [(E_1^0 - E_n^0) - E_1^0](rR_{n1}). \tag{6}$$

Using (6) we can show immediately that $u(r)$ satisfies

$$\left[E_1^0 + \frac{1}{2}\frac{d^2}{dr^2} + \left(\frac{1}{r} - \frac{1}{r^2}\right)\right]u(r) = \sum_{n\neq 1}^{\infty} rR_{n1}(r)\int_0^\infty R_{10}(r')R_{n1}(r')r'^3\, dr'.$$

Then, interchanging the order of summation and integration, and application of the closure relation for the $l = 1$ radial functions:

$$\sum_{n\neq 1}^{\infty} rR_{n1}(r)r'R_{n1}(r') = \delta(r - r')$$

gives us the differential equation satisfied by u:

$$\left[E_1^0 + \frac{1}{2}\frac{d^2}{dr^2} + \left(\frac{1}{r} - \frac{1}{r^2}\right)\right]u = r^2R_{10}(r) \tag{7}$$

which is equivalent to Schiff's Eq. (33.4). If we can find $u(r)$ then it is evident that

$$\Sigma = \int_0^\infty u(r)R_{10}(r)r^2\, dr = 2\int_0^\infty u(r)r^2e^{-r}\, dr. \tag{8}$$

Thus the summation reduces to the solution of Eq. (7) followed by the evaluation of the integral (8). However, the use of Laplace transforms avoids both steps.

We note that if we define the Laplace transform of $u(r)$:

$$v(p) = \int_0^\infty u(r)e^{-pr}\, dr \tag{9}$$

then

$$\Sigma = 2\left(\frac{d^2v}{dp^2}\right)_{p=1}. \tag{10}$$

Noting that $E_1^0 = -1/2$ in our units and rewriting Eq. (7) in the form

$$\left(\frac{r^2}{2}\frac{d^2}{dr^2} - \frac{r^2}{2} + r - 1\right)u = r^4R_{10} = 2r^4e^{-r}, \tag{11}$$

we find the Laplace transform of Eq. (11) is

$$\frac{1}{2}(p^2 - 1)\frac{d^2v}{dp^2} + (2p - 1)\frac{dv}{dp} = 48(1 + p)^{-5}, \tag{12}$$

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Calculation of the differential cross section for electron capture in fast ion-atom collisions

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The approach to electron capture developed by Chan and Eichler is combined with the optical eikonal approximation for describing the effect of the internuclear potential on the projectile trajectory. In this way, a closed-form expression is derived for the differential cross section for $1s \rightarrow nlm$ capture. Numerical calculations have been performed for the reaction $H^+ + H(1s) \rightarrow H + H^+$ at collision energies of 25, 60, and 125 keV. Good agreement is obtained with the recent data of Martin *et al.* by using trajectories undeflected by the internuclear potential at small deflection angles and Coulomb-deflected trajectories at large deflection angles.

I. INTRODUCTION

Measurements of differential capture cross sections present a much more stringent test of theory than experimental data on total cross sections. In earlier experiments[1] such measurements have been confined to collisions of protons with multielectron targets (He and Ar), and only very recently Martin *et al.*[2] have reported differential capture cross sections for the one-electron collision system $H^+ + H(1s)$ which offers the cleanest test for any theory. This may help to clarify the longstanding[3] problem of the role played by the internuclear potential[4,5] in theoretical approaches.

In the present work we adopt the eikonal approach developed by Chan and Eichler[6] (in the following denoted by CE in order to save the term "eikonal" for the optical description of the projectile trajectory). This approach, extended in further work,[7-9] has proven to be quite successful[6-9] in predicting total capture cross sections. Its results are expressed by simple formulas which are derived from the original ansatz without further approximations. The agreement with experiment (for collision velocities high enough with respect to typical electron orbital velocities in target and projectile) is based on the fact that the CE theory takes into account the interaction of the captured electron with both the projectile nucleus (in first order) and the target nucleus (in higher order) and thus approximately includes double and multiple scattering contributions. The physical content of the CE approach has been analyzed in more detail[10] by performing a term-by-term comparison with the Born expansion. It is worth mentioning at this point that exact second-Born calculations[11] at collision velocities close to, and a few times greater than, the electron orbital velocity yield capture cross sections which are up to an order of magnitude too large. This makes it clear that the third order and higher orders are needed[10] to bring the cross section down to the experimental value or to the value predicted by the nonperturbative CE theory.

In this paper we adopt the optical eikonal approximation[12] to describe the effect of the internuclear potential on the projectile trajectory and combine it with the CE approach[6] for calculating the transition amplitude for electron capture as a function of the impact parameter. In Sec. II we give a brief outline of the theory and in Sec. III apply the resulting formula to the collision system $H^+ + H(1s)$ in order to compare with the recent experimental results.

II. THEORY

Consider the capture of an electron initially bound in the $1s$ shell of a hydrogenic target with

PHYSICAL REVIEW A VOLUME 24, NUMBER 2 AUGUST 1981

Eikonal calculation of electron-capture cross sections from an arbitrary nlm shell of a hydrogenic target into an arbitrary $n'l'm'$ shell of a fast bare projectile

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Using techniques similar to those previously employed, we apply the eikonal approximation to the evaluation of the cross section for electron capture from an arbitrary nlm shell of a hydrogenic target atom into an arbitrary $n'l'm'$ of a fast hydrogenic projectile. The results are obtained in exact analytical closed form. Numerical results are presented for the case $H^+ + H(1s) \rightarrow H(n'l'm') + H^+$ when $n' = 2$ and 3. Comparison is made with the corresponding Oppenheimer-Brinkman-Kramers (OBK) results.

I. INTRODUCTION

Charge-transfer processes have been of interest since the early days of quantum mechanics. This interest has increased considerably in the past few years, the focus being on processes relevant to magnetically confined-fusion plasmas and astrophysical plasmas. Knowledge concerning the charge transfer from a hydrogenic atom to a bare ion is important not only with regard to these applications but also from a fundamental point of view since such a process is the simplest type of a rearrangement reaction.

An approach for treating electron capture into arbitrary principle shells of energetic projectiles based on the eikonal approximation was developed by Chan and Eichler.[1] They later amended their approach for capture into arbitrary n', l' sublevels of a fast projectile from the ground state[2] as well as from an arbitrary initial n, l sublevel[3] of a hydrogenic target. The results obtained agree well with experimental findings for hydrogen and helium targets. In this paper we extend the eikonal treatment to cover n, l, m contributions. There are at least two reasons why such a study is interesting. First of all, specification of these contributions allow for a sterner test of capture theories. Such a test is realizable since techniques for measuring charge exchange for $p + N_2 \rightarrow N_2^+ + H(n' = 3, l', m')$ have recently been developed[4] and a corresponding study of charge capture for $p + H$ collisions is now underway at Harvard University.[5] The present study is partly motivated by these experimental interests. Secondly, it is the most general case and it contains all the previous results[1-3] as special cases. In addition, it furnishes information not available from classical trajectory Monte Carlo calculations.[6]

In Sec. II, we use the eikonal approximation to calculate the cross section for the capture of an electron into an (n', l', m') state of an energetic projectile from a hydrogenic target initially in the (n, l, m) state. The result is obtained in closed form, and is exact within the eikonal approximation. In Sec. III, we discuss our results and present some theoretical data for the reaction $H^+ + H(1s) \rightarrow H(n' = 2, 3, l', m') + H^+$. The Oppenheimer-Brinkman-Kramers (OBK) results are obtained as a limiting case and are given in the Appendix.

II. THEORY

We consider the process in which an electron, initially in the n, l, m state of a hydrogenic target atom of charge Z_t, is captured into a given n', l', m' state of a bare projectile ion of charge Z_p. We assume that the time which the projectile spends in the vicinity of the target nucleus is small compared with the transition time of the electron. Let $\vec{r}$, $\vec{r}_t = \vec{r} + \alpha \vec{R}$, and $\vec{r}_p = \vec{r} - (1 - \alpha)\vec{R}$ denote the position of the electron with respect to the center of mass, the target nucleus, and the projectile nucleus, respectively, with $\alpha = M_p/(M_p + M_t)$. The projectile is supposed to move rectilinearly and that its trajectory is given by $\vec{R}(t) = \vec{b} + \vec{v}t$ ($\vec{b} \cdot \vec{v} = 0$, $|\vec{b}|$ being the classical impact parameter) with respect to the target nucleus. The cross section can then be written as[7]

$$\sigma_{nlm-n'l'm'}(v) = \int |A_{nlm-n'l'm'}(\vec{b}, v)|^2 d^2b , \quad (1)$$

where the exact eikonal transition amplitude is, in its "prior" form, given by

$$A_{nlm-n'l'm'}(\vec{b}, v) = -i \int_{-\infty}^{\infty} \left\langle \Psi_{n'l'm'} \left| -\frac{Z_p}{r_p} \right| \psi_{nlm} \right\rangle dt , \quad (2)$$

with the time-dependent wave functions

$$\psi_{nlm} = \varphi_{nlm}(\vec{r}_t) \exp(-i\epsilon_p t) \exp(-i\alpha \vec{v} \cdot \vec{r} - \tfrac{1}{2} i \alpha^2 v^2 t) \quad (3)$$

and

PHYSICAL REVIEW A VOLUME 24, NUMBER 6 DECEMBER 1981

Eikonal approximation for charge transfer from a multielectron atom to fast projectiles

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The eikonal approach developed previously for calculating electron-capture cross sections for bare projectiles colliding with hydrogenic targets is extended here to allow for multielectron targets. Both the impact and wave pictures are employed and their equivalence is discussed. As a first approximation, each atomic orbital is specified by the three hydrogenic quantum numbers, an effective nuclear charge Z_t, and an energy eigenvalue in the impact picture, or ionization potential in the wave picture. The Z_t' appearing in the eikonal phase factor is left undetermined because of incomplete information on the many-body target. However, analytic expressions are derived for the theoretical cross sections, and numerical values are calculated for simple choices of Z_t'. Those results are compared with existing experimental data for C, Ne, Ar, N_2, O_2, and He targets.

I. INTRODUCTION

Electron-capture processes in ion-atom collisions, e.g., $A^+ + B \rightarrow A + B^+$, are of great interest both in terms of basic theory and in various practical applications. In particular, a capture cross section from atomic oxygen or iron are essential in finding the charge equilibrium of a high-energy beam passing through different gases, or in finding the radiation of cosmic rays passing through interstellar matter.

It is well known that the Oppenheimer-Brinkman-Kramers (OBK) approximation[1] gives a roughly correct shape for the dependence of the total electron-capture cross sections upon the collision energy but considerably overestimates the observed data by as much as an order of magnitude. Many efforts have been devoted to obtain a simple semiempirical formula of the capture cross section by scaling down the OBK results through the comparison with the existing experimental measurements.[2] The physical significance of this scaling behavior was not quite understood until the very recent elegant and instructive illustration furnished by the study within the eikonal approximation.[3] This eikonal approach has been further studied since then and has been very successful in predicting the cross sections of the electron capture for the bare projectile—hydrogenic target systems.[4–8] Among them the cross sections of the capture (i) from nl initial state to $n'l'$ final state,[6] and (ii) from nlm initial state to $n'l'm'$ final state[8] have been obtained in closed form, a very astonishing consequence considering most of other approaches (other than OBK) are so complicated that one must have recourse to numerical methods.

In this paper, we generalize this eikonal approach to describe, in (i) the impact picture and (ii) the wave picture, the capture process of a single electron from a multielectron atom into a fast bare projectile. As a first approximation, each atomic orbital is specified by the three hydrogenic quantum numbers, an effective charge, and an energy value (more accurately, an energy eigenvalue in the impact picture or an ionization potential in the wave picture).

In Sec. II, two techniques in formulating the capture cross section are presented, i.e., (i) a straightforward extension from one of our recent papers[8] and (ii) a generating operator (a differential operator, or, for short, a differentiator) and a generating function (an exponential function) are introduced in manipulations. In Sec. III, a discussion on the equivalence of the wave and impact pictures is given. And finally, in Sec. IV, our calculations are compared with the existing experimental data for capture cross sections from C, Ne, Ar, N_2, O_2, and He.

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Applications of the Glauber and Eikonal Approximations to Atomic Collisions

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Comparison of the Born and Glauber generalized oscillator strengths for the $2s \rightarrow 3p$ transition of atomic hydrogen

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Minima and maxima of the generalized oscillator strength for the $2s \rightarrow 3p$ transition of atomic hydrogen are found using the Glauber approximation. In contrast to the first-Born approximation, the *number* of extrema and their positions are found to vary with the energy of the incident particle, and the values at the minima do not vanish. There is qualitative agreement in the behavior of the first minimum with known experimental data on the resonance transitions of rare gases and mercury. For large incident energy, the transition amplitude in the Glauber approximation falls off with large momentum transfer more rapidly than predicted by a previous calculation based on the second-Born approximation.

I. INTRODUCTION

The cross sections for discrete excitations often show undulations in the angular distributions. In the first-Born approximation (FBA) these undulations can be attributed to minima in the corresponding generalized oscillator strength (GOS). The minima in the GOS arise from a combination of the oscillations in the wave functions of the target atoms as well as oscillations in the transition operator.[1-4] Calculations based on the FBA have been verified *qualitatively* in many experiments,[2,5,6] and at very high incident energies the location of the minima are in agreement with experiment.[5] However, even at infinite energy, the FBA fails at very large momentum transfers,[7] partly because the FBA does not account for scattering by the nucleus at all.

In the FBA, the GOS is expressed as a function of the momentum transfer $\vec{K}$ (we use atomic units) and it is independent of the incident energy. Hence, the positions of the minima and maxima in the GOS remain fixed as incident energy is varied. The minima in the Born GOS occur when the transition matrix element changes sign, and therefore the GOS vanishes at the minima.

Experimental data, however, differ from the FBA results in three aspects: (a) the "experimental" GOS does not vanish at the minimum, (b) the magnitude of the GOS at the minimum depends on the incident energy, and (c) the position of the first minimum (expressed in terms of K) is shifted toward smaller K at intermediate- to low-incident-electron energies (<500 eV). Owing to the low intensity for large-angle scattering, subsequent minima at higher K have not been observed in any experiment so far. Another failure of the FBA is that the GOS falls off too rapidly as $K \rightarrow \infty$.[7]

In this paper, we present a study in the Glauber approximation of the minima in the GOS and the asymptotic behavior in K of the $2s \rightarrow 3p$ excitation of the hydrogen atom by electron impact.

Physically, there are several mechanisms that could produce the observed difference between the experimental and FBA results. In inelastic scattering the orthogonality of wave functions for the initial and final atomic states causes the nuclear-potential contribution to vanish in the FBA. In the second Born approximation (SBA), however, the nuclear potential is retained via coupling to the elastic channel in intermediate states. A recent estimate[8] of a part of the SBA amplitudes shows that SBA can partly account for the nonvanishing minima, and the positions of the minima shift with the incident energy. Furthermore, the SBA correction falls off more slowly with K and dominates over the FBA term at large K.

Another mechanism that could result in nonzero values of the minima is spin-orbit splitting. When the experimental resolution is insufficient to resolve multiplets split by the spin-orbit coupling, then the experimental minima may not vanish because each level of the multiplets may have minima at different K. Then the unresolved experimental data would appear as if there were one nonvanishing minimum. For instance, for the $6\,^2S \rightarrow 6\,^2P$ transition of Au, the spin-orbit interaction shifts slightly the locations of the zero minima for the spin-orbit doublet (see Table I). On the other hand, the effects of electron correlation shift the location of the minima, but they are not likely to change the fact that the FBA produces a zero minimum because the minimum (at least the major one) is a result of the vanishing transition ampli-

Plutonium-free bomb

I very much appreciated the article "Nuclear power and nuclear-weapons proliferation" by Ernest J. Moniz and Thomas L. Neff that appeared in the April issue (page 42). Of all the information I acquired in perusing the article, the most astonishing is the discovery, based upon the figure on page 44, of the extreme potency of plutonium as a bomb material. For, it would appear, one could reduce the fissile content of plutonium to 0% and still produce a bomb with a critical mass of 20 kg—a plutonium-free plutonium bomb!

I checked the reference cited in the figure caption. Only the points with fissile content $\geq 50\%$ are cited there, together with the information that the non-fissile material is plutonium 240 and 242. Surely the curve must rise to infinite critical mass as the fissile content falls to zero? Or am I so out of touch with this subject as to believe that fissile materials are essential to a fission bomb?

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Quantum mechanics in momentum space: An illustration

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The formulation of quantum-mechanical problems in momentum space, which is largely ignored in traditional courses but is used in research, is discussed. In particular, the formulation of scattering problems, for which the momentum representation is quite natural, is neither generally well known nor obvious. This is illustrated by solving a simple problem, the one-dimensional delta function potential, for which the bound state and continuum wave function are found.

I. INTRODUCTION

In traditional quantum mechanics courses,[1,2] students are exposed to a wide variety of problems, all of which are defined in configuration space (x representation). While momentum space (p representation) is generally introduced in a formal way,[3] it is rarely used in the solution of problems.[4] Any momentum space functions which are needed are generally derived by solving the problem in the x representation and then Fourier transforming the result. This is no doubt because the potential function in configuration space becomes an integral operator in momentum space and the Schrödinger equation becomes an integral equation. However, for many problems the momentum representation is actually more natural. This is particularly true in scattering problems, where one is interested in calculating the probability amplitude for the change in direction of the momentum vector. In fact, in the usual treatment of potential scattering found in textbooks,[5] the Schrödinger equation is converted into an integral equation by means of the free particle Green's function, and the latter is found by means of Fourier transformation. This technique is in effect utilizing the simple form of the free Green's function in momentum space, where the kinetic energy operator is diagonal. Since the x-space and p-space equations are both integral equations, the advantage of the former would appear to be lost. Other arguments for using the p representation have been given by Dirac in his classic text.[6]

It is the purpose of this paper to illustrate the solution of the Schrödinger equation in momentum space by means of a simple example for which the configuration space solution is relatively familiar: the one-dimensional motion of a particle in a delta function potential.[7] While this potential may not be physically realistic, most of the characteristics of the Schrödinger equation may be illustrated by its use, and so it is of pedagogical value.

II. SCHRÖDINGER EQUATION IN MOMENTUM SPACE

We begin with the Schrödinger equation in the x representation

$$(E-\hat{p}^2/2m)\psi(x)=V(x)\psi(x), \tag{1}$$

where $\hat{p}$ represents the operator $-i\hbar\, d/dx$. The momentum space wave function $\phi(p)$ is defined by

$$\phi(p)=(2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty}\exp(-ipx/\hbar)\psi(x)\,dx \tag{2}$$

with the inverse relation

$$\psi(x)=(2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty}\exp(ipx/\hbar)\phi(p)\,dp. \tag{3}$$

The function $\phi(p)$ plays the same role in the p representation that $\psi(x)$ plays in x space; for example, the probability that a measurement of the momentum will fall between p and $p+dp$ is given by $|\phi(p)|^2\,dp$. In terms of $\phi(p)$ the Schrödinger equation, Eq. (1), becomes an integral equation:

$$(E-p^2/2m)\phi(p)=(2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty}\tilde{V}(p-p')\phi(p')\,dp'. \tag{4}$$

In this equation p is merely a *number* (the kinetic energy operator, like the momentum, is diagonal in the p representation), while $\tilde{V}(p-p')$ is, apart from the occurrences of $\hbar$, the Fourier transform of $V(x)$:

$$\tilde{V}(p)=(2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty}\exp(-ipx/\hbar)V(x)\,dx. \tag{5}$$

In this paper we shall take for illustrative purposes the potential

$$V(x)=c\delta(x), \tag{6}$$

where c is a constant of dimension energy times length. For this potential we have

$$\tilde{V}(p)=(2\pi\hbar)^{-1/2}c, \tag{7}$$

and Eq. (4) takes the particularly simple form

$$(E-p^2/2m)\phi(p)=(c/2\pi\hbar)\int_{-\infty}^{\infty}\phi(p)\,dp. \tag{8}$$

The Complete Asymptotic Expansion of the Continuum Schrödinger Wave Function

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A complete asymptotic expansion, in inverse powers of the distance, for the scattered wave function solution to Schrödinger's equation with a short-range potential is derived by two simple arguments. The result is identical to a more rigorous calculation by Buslaev. The difference between the asymptotic series and the exact wave function vanishes at infinity faster than any negative power of the distance. Explicit formulas for the coefficients are derived and their physical significance discussed. The application to the uniqueness theorem for the Schrödinger equation is also discussed.

I. INTRODUCTION

The scattering of two particles which interact by means of a potential $V(\mathbf{r})$ is described (in center-of-mass coordinates) by a wave function $\psi(\mathbf{r})$ satisfying the Schrödinger equation

$$[\nabla^2+k^2-U(\mathbf{r})]\psi(\mathbf{r})=0. \tag{1}$$

In this equation we have put

$$U(\mathbf{r})=2\mu V(\mathbf{r})/\hbar^2 \tag{2}$$

and the center-of-mass energy

$$E=\hbar^2k^2/2\mu \tag{3}$$

where μ is the reduced mass of the particles. It is shown in most graduate-level quantum mechanics textbooks[1] that Eq. (1) has a solution of the form

$$\psi(\mathbf{r})=\psi_k(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})+\tilde{\psi}_k(\mathbf{r}) \tag{4}$$

where the "scattered" part of the wave function $\tilde{\psi}_k$ satsifies the outgoing wave boundary condition

$$\tilde{\psi}_k(\mathbf{r})\sim r^{-1}\exp(ikr)f_k(\hat{\mathbf{r}}) \tag{5}$$

as $r\to\infty$ in the direction of the unit vector $\hat{\mathbf{r}}$.[2] The scattering amplitude $f_k(\hat{\mathbf{r}})$ is related to ψ_k by

$$f_k(\hat{\mathbf{r}})=-(4\pi)^{-1}\int\exp(-ik\hat{\mathbf{r}}\cdot\mathbf{r}')U(\mathbf{r}')\psi_k(r')d^3r'. \tag{6}$$

The derivation of these results[1] proceeds by converting Eq. (1) into an integral equation incorporating the boundary condition at infinity, Eqs. (4)–(5):

$$\psi_k(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})+\int G_k(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi_k(\mathbf{r}')d^3r' \tag{7}$$

where the free Green's function G_k is given by

$$G_k(\mathbf{r},\mathbf{r}')=-(4\pi)^{-1}\exp(ik|\mathbf{r}-\mathbf{r}'|)/|\mathbf{r}-\mathbf{r}'|. \tag{8}$$

The demonstration that Eqs. (7)–(8) do indeed incorporate Eq. (5) with f_k given by Eq. (6) follows by expanding G_k in the region $r\gg r'$, which is justified if $U(\mathbf{r}')$ falls off rapidly at infinity (since ψ_k must be bounded), with the result that the G_k appearing in Eq. (7) is replaced by its asymptotic expression

$$G_k(r,r')\sim-(4\pi r)^{-1}\exp(ikr)\exp(-ik\hat{\mathbf{r}}\cdot\mathbf{r}'). \tag{9}$$

It is evident from this discussion that Eq. (5) represents only the first term in an asymptotic development of the scattered wave function $\tilde{\psi}_k$ of the form [for well behaved $V(\mathbf{r})$]

$$\tilde{\psi}_k(\mathbf{r})\sim(e^{ikr}/r)\sum_{j=0}[g_j(\hat{\mathbf{r}})/r^j]. \tag{10}$$

The coefficient g_0 is just f_k and the higher co-

Variational Principles for Three-Body Breakup Scattering

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In the preceding paper we derived a Kohn-type variational principle for the scattering amplitude for the breakup of a bound pair by an incident third particle. In this paper an alternative derivation is presented. The new derivation, based on the Faddeev equations, though rather formal, is rigorous; the preceding derivation was not. This procedure sheds some light on the manipulations in the earlier derivation. We also derive an "adjoint" Kohn-type variational principle in which the operator $H-E$ acts on the final-state wave function. The "adjoint" result has some convergence difficulties but these have been overcome by techniques described. Finally, a Schwinger-type variational principle is derived and its connection with the recently proposed variational principle of Pieper, Schlessinger, and Wright is discussed.

I. INTRODUCTION

In the preceding paper[1] we presented a Kohn-type variational principle for the scattering amplitude for the breakup of a bound pair by an incident third particle.[2] The derivation was to some extent heuristic. We found it necessary at intermediate stages to introduce divergent integrals which arose because we did not know how to avoid interchanging the order of a spatial integration and a limiting process onto the real energy axis. We demonstrated that these integrals could be treated by introducing a procedure which we call "radius averaging," an analog for integration of the techniques of Cesàro summation. Since the integrals needed for applications are not divergent, ordinary integration techniques suffice in the final form.

In the present paper we first present a rigorous proof of the above variational principle, which is based upon the Faddeev equations.[3] This proof, while quite formal in nature, avoids some of the difficulties of the previous derivation and lends greater credibility to the procedures introduced there. In particular, it is possible in the new derivation to work entirely with real energies so that the question of the order of limit and integral does not arise; radius averaging is still used as a convenient (but now fully justified) technical device.

In Sec. III we present an "adjoint" variational principle of the Kohn type for the breakup amplitude, in which the roles of the initial- and final-state wave functions are interchanged. This principle, in contrast to the direct version, requires radius averaging in its final form if we use rudimentary trial wave functions. We show, however, that there exists an alternative to the radius-averaging procedure, if one knows the exact two-body on-shell scattering amplitudes; one may easily incorporate these exact amplitudes into the trial functions in such a way as to have only convergent integrals. Either way this principle may be a useful complement to the direct form.

Finally, we discuss variational principles of the Schwinger type.[4] It is well known that the Schwinger principle for two-body scattering may be obtained from the Kohn principle by using a trial function constructed by an iteration of the Kohn trial function in the Lippmann-Schwinger equation. When an analogous procedure is applied in the present case we find that in general radius averaging is required to define individual terms in the variational expression. However, by explicitly including some exact two-body portions of the final-state trial function and by combining terms appropriately the final form may be made completely convergent. A single further step reproduces the variational principle recently proposed by Pieper *et al.*[5] The starting point of this analysis can be taken to be any one of the three Kohn-type principles derived here [see Eqs. (2.36), (2.41), and (3.6)]. This is shown in Sec. IV, with additional details in an Appendix. Section IV concludes with some comparisons between the Kohn-type principle and the variational principle of Pieper *et al.*

Throughout this paper, we use the notation of I.

II. THE FADDEEV-EQUATION DERIVATION OF THE KOHN VARIATIONAL PRINCIPLE

In our previous paper[1] we derived a variational expression for the breakup amplitude in the Kohn

NOTES AND DISCUSSIONS

An Operator Domain Paradox and the Relativistic Correction to Energy Levels

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It has been frequently emphasized[1] that proper caution must be exercised in dealing with the unbounded operators occurring in quantum mechanics in order to avoid error and confusion. In particular, the domain on which an operator is defined may be larger than the domain on which it is Hermitian.[2] The purpose of this note is to point out that a striking example of this apparently anomalous behavior occurs in a quite familiar and practical problem about which false or misleading statements exist in the literature.

As the square of the Hermitian operator p^2, the operator p^4 should have only *positive* expectation values. On the other hand, if we replace the expression $(\psi_0, p^4\psi_0)$ by $(p^2\psi_0, p^2\psi_0)$, we obtain

$$\begin{aligned}(p^2\psi_0, p^2\psi_0) &= (2m)^2\{[E_0+(e^2/r)]\psi_0, [E_0+(e^2/r)]\psi_0\}\\ &= (2m)^2\{\psi_0, [E_0+(e^2/r)]^2\psi_0\}\\ &= 5(\hbar/a_0)^4 = 5(\alpha mc)^4,\end{aligned} \tag{7}$$

where $E_0=-e^2/2a_0$ is the unperturbed ground-state energy and $\alpha=e^2/\hbar c=1/137$. The result Eq. (7), is more palatable than Eq. (6) and leads to a shift

$$\Delta E=-\tfrac{5}{8}\alpha^4 mc^2 \tag{8}$$

which agrees with the corresponding "exact" result obtained from an expansion of the Klein-Gordon energy[6,7] in powers of α.

The origin of the difficulty is evidently that, while ψ_0