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Position-operator method for evaluating the shift of a totally reflected electron

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A method based on expectation values of a position operator is developed for evaluating the spatial shift of a polarized Dirac electron undergoing total reflection. Longitudinal and transverse components of the shift, as well as the associated time delay, are obtained by considering the differences in the expectation values for the physically reflected wave packet and a purely geometrically reflected wave packet. For a number of position operators, this method is used to calculate the mean shift arising from a single reflection of an electron from a step-function potential. Eigenpolarization states are determined by means of a localization form-invariance argument. For these states, results obtained employing the Newton-Wigner position operator are shown to be identical to those obtained using the phase-shift analysis method. A comparison calculation giving different results is made using the current-flux method. The current-flux results are shown to be inconsistent with conservation of total angular momentum normal to the reflecting boundary.

I. INTRODUCTION

It has been demonstrated experimentally[1] that a well-collimated light beam undergoes a spatial shift (the Goos-Hänchen effect) when it is totally reflected. In general, for such a shift to be observable, an experimental arrangement producing a series of total reflections is required. The type of shift observed depends both on the polarization of the incident beam and the geometrical arrangement of the reflecting surfaces. Although the experimental evidence is unambiguous, the theoretical explanation has followed several approaches, each of which yields a somewhat different prediction. Basically, these approaches have involved either a phase-shift analysis method[2] (applied to a single-surface reflection process or a multiple-surface reflection process) or a current-flux method[3] (applied to a single-surface reflection process).

For particles undergoing total reflection, it has been predicted that similar spatial shifts should occur.[4,5] Again, the theory has followed the two main lines mentioned above. Recently,[6] we have presented a variant of the phase-shift method in order to predict the spatial shift for a polarized Dirac electron undergoing a series of total reflections. Localization of the electron has been taken into account explicitly via a wave-packet treatment, and a localization form-invariance argument has been given to determine the eigenpolarization states for a multiple-reflection process and the relevant phase shifts.

In the present paper we develop another method, based on expectation values of a position operator, for the evaluation of the spatial shift that would occur in the position of a polarized Dirac electron undergoing total reflection. Longitudinal and transverse components of this shift, as well as the associated time delay, are obtained by considering the differences in the expectation values for the physically reflected wave packet and a purely geometrically reflected wave packet. In order to facilitate comparison with the results obtained by other techniques, we restrict our attention to a single-surface process, although the position-operator method may be generalized to treat a multiple-surface process.

The organization of this paper is the following. In Sec. II, we present the solution of the Dirac equation for a polarized positive-energy state totally reflecting from a step-function potential. In addition, we evaluate the current densities for the incident, reflected, and evanescent components of the solution. In Sec. III, we determine the eigenpolarization states for a single-reflection process, and calculate the spatial shift and time delay by the phase-shift analysis method utilizing a localization form-invariance argument. In Sec. IV we develop the general formulation of an expectation-value calculation of the shifts involving a position operator. The results obtained for the Newton-Wigner position operator and other position operators are presented and compared with the results previously obtained via the phase-shift method. In Sec. V, the current-flux method is used to evaluate the shifts, and further comparisons are made. Finally, in Sec. VI, the current-flux method is criticized on the basis of symmetry considerations.

II. SOLUTION OF THE DIRAC EQUATION FOR A STEP-FUNCTION POTENTIAL

In this section we shall collect and reorganize results from an earlier paper[6] dealing in part with

the total reflection of a polarized electron from a step-function potential discontinuity. For $x_3 < 0$, the appropriate solution of the Dirac equation

$$[\vec{\alpha}\cdot\vec{p} + \beta m + V_0\theta(x_3)]\psi = E\psi \tag{1}$$

is the superposition of the incident wave

$$\psi^I(\vec{p}, \hat{s}) = e^{i(\vec{p}\cdot\vec{x} - Et)}\psi(\vec{p}, \hat{s}) \tag{2}$$

and the reflected wave

$$\psi^R(\vec{p}', \hat{s}') = e^{i(\vec{p}'\cdot\vec{x} - Et)}e^{-i\delta(\vec{p})}e^{-i\chi(\vec{p}, \hat{s})}\psi(\vec{p}', \hat{s}'), \tag{3}$$

where the normalized spinor $\psi(\vec{p}, \hat{s})$ has the form

$$\psi(\vec{p}, \hat{s}) = [2E(E+m)]^{-1/2}\begin{pmatrix} (E+m)\,\Phi(\hat{s}) \\ \vec{\sigma}\cdot\vec{p}\;\;\Phi(\hat{s}) \end{pmatrix}. \tag{4}$$

Here $\hat{s}$ is the direction of polarization of the incident wave, and $\Phi(\hat{s})$ is the two-component eigenfunction of $\vec{\sigma}\cdot\hat{s}$ given by

$$\Phi(\hat{s}) = \begin{pmatrix} \cos\tfrac{1}{2}\theta_s & e^{-i\phi_s/2} \\ \sin\tfrac{1}{2}\theta_s & e^{i\phi_s/2} \end{pmatrix}, \tag{5}$$

where θ_s and ϕ_s are the polar and azimuthal angles of $\hat{s}$. The momentum of the reflected wave is

$$\vec{p}' = \vec{p} - 2(\vec{p}\cdot\hat{x}_3)\hat{x}_3, \tag{6}$$

and the polarization of the reflected wave is

$$\hat{s}' = (\hat{s}_t\cdot\hat{s})\hat{s}_t + [\sin\gamma(\vec{p})]\,\hat{s}\times\hat{s}_t + [\cos\gamma(\vec{p})]\,\hat{s}_t\times(\hat{s}\times\hat{s}_t), \tag{7}$$

where

$$\hat{s}_t = (\vec{p}\times\hat{x}_3)/\rho \tag{8}$$

and where

$$\exp[i\tfrac{1}{2}\gamma(\vec{p})] = (E+m)^{-1}(E^2 - p_3^2)^{-1/2} \times[(E^2 - p_3^2 + mE) + i\rho p_3]. \tag{9}$$

For convenience we have defined $\rho \equiv |\vec{p}\times\hat{x}_3|$. The reflected polarization direction $\hat{s}'$ is produced by a clockwise precession (without nutation) of the incident polarization direction about $\hat{s}_t$ through an angle $\gamma(\vec{p})$.

In Eq. (3), the polarization-independent phase factor is

$$\delta(\vec{p}) = \arctan[\kappa p_3/(p_3^2 - EV_0)], \tag{10}$$

where the evanescent damping factor κ is defined by

$$\kappa^2 = p_1^2 + p_2^2 + m^2 - (E - V_0)^2. \tag{11}$$

The polarization-dependent phase factor is given by

$$e^{-2i\chi(\vec{p}, \hat{s})} = \frac{[\cos\gamma\sin\theta_s + \sin\gamma\cos\theta_s\cos(\phi_s - \phi)] - i[\sin\gamma\sin(\phi_s - \phi)]}{\{[\cos\gamma\sin\theta_s + \sin\gamma\cos\theta_s\cos(\phi_s - \phi)]^2 + [\sin\gamma\sin(\phi_s - \phi)]^2\}^{1/2}}, \tag{12}$$

where ϕ is the azimuthal angle of the momentum $\vec{p}$, and the functional dependence of γ has been suppressed.

For $x_3 > 0$, the solution is the evanescently transmitted wave

$$\psi^T(\kappa, \hat{s}) = e^{i(p_1x_1 + p_2x_2 - Et)}e^{-\kappa x_3}p_3[2/(V_0E)]^{1/2} \times e^{-i\delta(\vec{p})}\Phi(\kappa, \hat{s}). \tag{13}$$

Here the normalized spinor $\Phi(\kappa, \hat{s})$ is given by

$$\Phi(\kappa, \hat{s}) = [2(E - V_0 + m)(E^2 - p_3^2)^{1/2}]^{-1/2} \times \begin{pmatrix} (E - V_0 + m)U(\hat{s}_t)\Phi(\hat{s}) \\ \vec{\sigma}\cdot[\vec{p} - (p_3 - i\kappa)\hat{x}_3]\,U(\hat{s}_t)\Phi(\hat{s}) \end{pmatrix}, \tag{14}$$

where

$$U(\hat{s}_t) = [2V_0(E - V_0 + m)(E + m)(E^2 - p_3^2)^{1/2}]^{-1/2} \times[p_3(E - V_0 + m) + i\kappa(E + m) + i\rho V_0\vec{\sigma}\cdot\hat{s}_t]. \tag{15}$$

The matrix $U(\hat{s}_t)$ represents a "rotation" about the axis $\hat{s}_t$ through a complex angle $\tilde{\gamma}$, where

$$\tan(\tfrac{1}{2}\tilde{\gamma}) = \rho V_0/[p_3(E - V_0 + m) + i\kappa(E + m)]. \tag{16}$$

A. Current densities

The current-flux method to be discussed in Sec. V involves the use of plane-wave current densities. If ψ represents one of the wave-function contributions (incident, reflected, or transmitted), then the associated current density is

$$\vec{J} = \psi^\dagger\vec{\alpha}\psi, \tag{17}$$

where $\vec{\alpha}$ is the usual set of Dirac matrices. For the incident and reflected waves the current densities reduce to the associated velocities, i.e., $\vec{p}/E$ and $\vec{p}'/E$ for the incident and reflected waves, respectively.

On the evanescent side, it is convenient to decompose the current operators into longitudinal (L which denotes the longitudinal component measured in a plane parallel to the boundary plane) and transverse (t) components. These are defined by

$$\alpha_L = \vec{\alpha}\cdot\hat{x}_3\times\hat{s}_t \tag{18}$$

and

$$\alpha_t = \vec{\alpha}\cdot\hat{s}_t\,, \tag{19}$$

where $\hat{s}_t$ is defined in Eq. (8). Using these definitions and the transmitted wave function given in Eq. (13), one obtains the associated evanescent current densities

$$J_L = \frac{e^{-2\kappa x_3}\,2p_3^{\,2}}{EV_0(E^2-p_3^{\,2})}\,[\rho(E-V_0)-m\kappa(\hat{s}\cdot\hat{s}_t)] \tag{20}$$

and

$$J_t = \frac{e^{-2\kappa x_3}\,2\kappa p_3^{\,2}}{EV_0(E^2-p_3^{\,2})(E+m)} \times[(E^2-p_3^{\,2}+Em)(\hat{x}_3\times\hat{s}_t\cdot\hat{s})+\rho p_3(\hat{x}_3\cdot\hat{s})]\,. \tag{21}$$

The evanescent-current density component associated with the current operator $\vec{\alpha}\cdot\hat{x}_3$ is zero.

B. Foldy-Wouthuysen transformation

Some of the calculations performed later involving incident and reflected wave-packet expectation values are conveniently done in the Foldy-Wouthuysen (FW) representation.[7] The transformed wave function $\Psi_{\rm FW}$ and the generic operator $A_{\rm FW}$ are related to the corresponding quantities in the Dirac representation by

$$\Psi_{\rm FW} = e^{iS}\,\psi_{\rm Dirac}\,, \quad A_{\rm FW} = e^{iS}A_{\rm Dirac}\,e^{-iS}\,, \tag{22}$$

where the transformation operator e^{iS} is given by

$$e^{iS} = [2E(E+m)]^{-1/2}\,(\beta\vec{\alpha}\cdot\vec{p}+E+m)\,. \tag{23}$$

In the FW representation, the transform of the spinor $\psi(\vec{p},\hat{s})$ displayed in Eq. (4) assumes the especially simple form

$$e^{iS}\,\psi(\vec{p},\hat{s}) = \begin{pmatrix}\Phi(s)\\ 0\end{pmatrix}. \tag{24}$$

III. PHASE-SHIFT ANALYSIS

One method for calculating the displacement of an electron undergoing total reflection from a single surface involves the determination of the net phase shift, for a localized wave packet, that is characteristic of the reflection process. The relevant phase shifts and the associated eigenstates may be determined by means of a localization form-invariance argument similar to that used in a previous paper[6] concerned with multiple total reflections. In this section we shall adopt this argument to a single-surface reflection by reformulating for a step-function potential a wave-packet description employed by Miller and Ashby.[5]

In a coordinate system $\hat{X}_1, \hat{X}_2, \hat{X}_3$, which is aligned so that $\hat{X}_3$ is in the direction $(\vec{p}_0)$ of the incident electron, the incident wave packet has the form

$$\Psi^{\rm inc}(\vec{X},t) = (2\pi)^{-3/2}\int f(\vec{P}-\vec{p}_0,\hat{S})e^{i(\vec{P}\cdot\vec{X}-Et)} \times\psi(\vec{P},\hat{S})d^3P\,. \tag{25}$$

The weighting function $f(\vec{P}-\vec{p}_0,\hat{S})$, which is symmetric in both P_1 and P_2, has been chosen so that the packet is peaked about a single central position that moves in time with a velocity $\vec{p}_0/(m^2+p_0^{\,2})^{1/2}$.

The coordinate system $\hat{x}_1, \hat{x}_2, \hat{x}_3$, for which $\hat{x}_3$ is normal to the reflecting boundary and $\vec{p}_0$ is in the $\hat{x}_1$-$\hat{x}_3$ plane, is related to the $\hat{X}$ coordinate system by $\hat{x} = R_2(\theta_0)\hat{X}$. Explicitly,

$$\begin{pmatrix}\hat{x}_1\\ \hat{x}_2\\ \hat{x}_3\end{pmatrix} = \begin{pmatrix}\cos\theta_0 & 0 & -\sin\theta_0\\ 0 & 1 & 0\\ \sin\theta_0 & 0 & \cos\theta_0\end{pmatrix}\begin{pmatrix}\hat{X}_1\\ \hat{X}_2\\ \hat{X}_3\end{pmatrix}, \tag{26}$$

in which θ_0 is the angle between $\vec{p}_0$ and $\hat{x}_3$. In terms of this coordinate system, the incident wave packet is described by

$$\Psi^{\rm inc}(\vec{x},t) = (2\pi)^{-3/2}\int f(\vec{P}-\vec{p}_0,\hat{S})e^{i(\vec{p}\cdot\vec{x}-Et)} \times e^{-i\Delta(-\theta_0,\hat{s})}\psi(\vec{p},\hat{s})d^3P\,. \tag{27}$$

Here the components of the vectors $\vec{x}$, $\vec{p}$, and $\hat{s}$, are related to the components of the vectors $\vec{X}$, $\vec{P}$, and $\hat{S}$, by the coordinate transformations $x = R_2(-\theta_0)X$, etc. The phase factor $\Delta(-\theta_0,\hat{s})$ introduced by the spinor rotation is given by

$$e^{-2i\Delta(-\theta_0,\hat{s})} = \frac{(\sin\theta_s\cos\theta_0-\sin\theta_0\cos\phi_s\cos\theta_s)+i\sin\theta_0\sin\phi_s}{[(\sin\theta_s\cos\theta_0-\sin\theta_0\cos\phi_s\cos\theta_s)^2+(\sin\theta_0\sin\phi_s)^2]^{1/2}}\,. \tag{28}$$

After being totally reflected, the packet will have the form

$$\Psi^{\rm refl}(\vec{x},t) = (2\pi)^{-3/2}\int f(\vec{P}-\vec{p}_0,\hat{S})e^{i(\vec{p}'\cdot\vec{x}-Et)} \times e^{-i\Delta(-\theta_0,\hat{s})}e^{-i\delta(\vec{p})} \times e^{-i\chi(\vec{p},\hat{s})}\psi(\vec{p}',\hat{s}')d^3P\,, \tag{29}$$

where $\hat{s}'$ is the precessed polarization direction given by Eq. (7), $\delta(\vec{p})$ and $\chi(\vec{p},\hat{s})$ are the phase factors given by Eqs. (10) and (12), and $\vec{p}'$ indicates the momentum components of the reflected wave as given by Eq. (6). In terms of a coordinate system $\hat{X}_1'$, $\hat{X}_2'$, $\hat{X}_3'$ which is aligned so that $\hat{X}_3'$ is in the direction $\vec{p}_0'$ of the reflected electron, the

reflected wave packet is described by

$$\Psi^{\text{refl}}(\vec{X}', t) = (2\pi)^{-3/2}\int f(\vec{P}-\vec{p}_0, \hat{S}) e^{i(\vec{P}'\cdot\vec{X}'-Et)} \times e^{-i\eta}\psi(\vec{P}', \hat{S}')d^3P, \quad (30)$$

where here the components of the vectors $\vec{X}'$, $\vec{P}'$, and $\hat{S}'$ are related to the components of the vectors $\vec{x}$, $\vec{p}'$, and $\hat{s}'$ by the coordinate transformation $X' = R_2(\pi-\theta_0)x$, etc. The rotation matrix $R_2(\pi-\theta_0)$ about the 2 axis through an angle $\pi-\theta_0$ is obtained from Eq. (26) by making the suitable substitution of angles. The composite phase factor η is given by

$$\eta = \delta(\vec{p}) + \chi(\vec{p}, \hat{s}) + \Delta(-\theta_0, \hat{s}) + \Delta(\pi-\theta_0, \hat{S}'), \quad (31)$$

where $\Delta(\pi-\theta_0, \hat{S}')$ is obtained from Eq. (28) by replacing θ_0 by $\theta_0-\pi$, and θ_s, ϕ_s by $\theta_{S'}$, $\phi_{S'}$ which are the polar and azimuthal angles of the precessed polarization direction with respect to the $\hat{X}'$ coordinate system (i.e., measured with respect to $\hat{X}_3'$ and $\hat{X}_1'$, respectively).

Now, as a result of the coordinate transformations and the reflection,

$$\vec{P}' = -P_1\hat{X}_1' + P_2\hat{X}_2' + P_3\hat{X}_3', \quad (32)$$

where $\vec{P} = P_1\hat{X}_1 + P_2\hat{X}_2 + P_3\hat{X}_3$. Thus, since $f(P-p_0, S)$ is a scalar symmetric in both P_1 and P_2, the reflected wave packet displayed in Eq. (30) without the phase factor $e^{-i\eta}$ would have exactly the same form as the incident packet [displayed in Eq. (25)] if the components of $\hat{S}'$ were related to those of $\hat{S}$ by

$$\hat{S}' = S_1\hat{X}_1' + S_2\hat{X}_2' + S_3\hat{X}_3', \quad (33)$$

where $\hat{S} = S_1\hat{X}_1 + S_2\hat{X}_2 + S_3\hat{X}_3$. For those polarization directions, designated as the eigenpolarization directions, such that this condition (Eq. 33) of form invariance is satisfied, the reflected wave packet is peaked about a single central position that moves in time with a velocity $\vec{p}_0'/(m^2+p_0^2)^{1/2}$.

Solving Eq. (33) for the eigenpolarization directions, we find that the corresponding directions $\pm\hat{s}_e$ for the incident wave packet are given by

$$\hat{s}_e = (1-B^2)^{1/2}\begin{pmatrix} \sin\phi\sin\theta_0\sin\frac{1}{2}\gamma \\ \cos\theta_0\cos\frac{1}{2}\gamma - \cos\phi\sin\theta_0\sin\frac{1}{2}\gamma \\ \sin\phi\cos\theta_0\sin\frac{1}{2}\gamma \end{pmatrix}, \quad (34)$$

where the components are displayed in the $\hat{X}_1$, $\hat{X}_2$, $\hat{X}_3$ basis, and where

$$B = (\cos\phi\cos\theta_0\sin\tfrac{1}{2}\gamma + \sin\theta_0\cos\tfrac{1}{2}\gamma).$$

The components of $\hat{s}_e$ are related by

$$(\hat{s}_e)_3 = (\tan\tfrac{1}{2}\gamma)[(\hat{s}_e)_1\cos\phi + (\hat{s}_e)_2\sin\phi], \quad (35)$$

and the precessed polarization direction $\hat{s}_e'$ turns out to be $\hat{s}_e - 2(\hat{s}_e\cdot\hat{x}_3)\hat{x}_3$, which means that the eigenpolarization directions reverse upon reflection the same way the momentum does. Also, $\hat{s}_e\cdot\hat{X}_1$ is zero, which means that $(\hat{S}_e)_1$ is zero.

The composite phase factor contributions assume a somewhat simpler form for the eigenpolarization states. Defining

$$A = (1-B^2)^{1/2}[(\hat{s}_e)_2\cos\phi - (\hat{s}_e)_1\sin\phi] = \cos\theta_0\cos\phi\cos\tfrac{1}{2}\gamma - \sin\theta_0\sin\tfrac{1}{2}\gamma, \quad (36)$$

we find that

$$e^{-i\chi(\vec{p}, \pm\hat{s}_e)} = \frac{(1-B^2)^{1/2}\cos\frac{1}{2}\gamma \mp iA\sin\frac{1}{2}\gamma}{[(1-B^2)\cos^2(\frac{1}{2}\gamma) + A^2\sin^2(\frac{1}{2}\gamma)]^{1/2}}, \quad (37)$$

and

$$e^{-2i\Delta(-\theta_0, \pm\hat{s}_e)} = -e^{-2i\Delta(\pi-\theta_0, \pm\hat{s}_e')} = \frac{(\hat{s}_e\times\hat{x}_3)\cdot(\hat{s}_e\times\hat{X}_3) \pm i\hat{s}_e\cdot\hat{x}_3\times\hat{X}_3}{\{[(\hat{s}_e\times\hat{x}_3)\cdot(\hat{s}_e\times\hat{X}_3)]^2 + (\hat{s}_e\cdot\hat{x}_3\times\hat{X}_3)^2\}^{1/2}}. \quad (38)$$

The trajectory of the reflected wave packet may now be obtained from Eq. (30) by application of the method of stationary phase. Since $\vec{P}'\cdot\vec{X}' = \vec{p}'\cdot\vec{x}$, this method yields the result

$$\vec{x}^{\text{refl}} - (\vec{p}_0'/E)t - \vec{\nabla}_{p'}\eta = 0, \quad (39)$$

where $\vec{p}'$ and $\vec{p}$ are evaluated at $\vec{p}_0'$ and $\vec{p}_0$, respectively. Using the relations

$$\vec{p}'\times\hat{x}_3\cdot\vec{\nabla}_{p'} = \vec{p}\times\hat{x}_3\cdot\vec{\nabla}_p,$$

$$(\vec{p}'\times\hat{x}_3)\times\vec{p}'\cdot\vec{\nabla}_{p'} = \vec{p}\times(\vec{p}\times\hat{x}_3)\cdot\vec{\nabla}_p,$$

and

$$\vec{p}'\cdot\vec{\nabla}_{p'} = \vec{p}\cdot\vec{\nabla}_p,$$

Eq. (39) for the reflected wave-packet trajectory may be rewritten

$$\vec{x}^{\text{refl}} = (t-\tau)(\vec{p}_0'/E) + D_t\frac{\vec{p}'\times\hat{x}_3}{|\vec{p}'\times\hat{x}_3|} + D_l\frac{(\vec{p}'\times\hat{x}_3)\times\vec{p}'}{p|\vec{p}'\times\hat{x}_3|}. \quad (40)$$

Here the time delay τ is given by

$$\tau = -(E/p^2)[\vec{p}\cdot\vec{\nabla}_p\eta(\vec{p}, \pm\hat{s}_e)], \quad (41)$$

and the transverse shift D_t and the longitudinal shift D_l are given by

$$D_t = \rho^{-1}[\vec{p}\times\hat{x}_3\cdot\vec{\nabla}_p\eta(\vec{p}, \pm\hat{s}_3)] \quad (42)$$

and

$$D_l = (\rho p)^{-1}[\vec{p}\times(\vec{p}\times\hat{x}_3)\cdot\vec{\nabla}_p\eta(\vec{p}, \pm\hat{s}_3)]. \quad (43)$$

Upon substitution of the relevant derivatives of the composite phase factor for the eigenpolariza-

tions $\pm \hat{s}_e$, we obtain

$$\tau(\pm \hat{s}_e) = \frac{p_3[m^2(E-V_0)+E(E^2-p_3^2)]}{\kappa(E^2-p_3^2)p^2} \mp \frac{\rho p_3 m}{(E^2-p_3^2)p^2}, \tag{44}$$

$$D_t(\pm \hat{s}_e) = 0, \tag{45}$$

and

$$D_l(\pm \hat{s}_e) = \frac{\rho(2E^2-p_3^2-EV_0)}{\kappa p(E^2-p_3^2)} \pm \frac{(Em+p_3^2-E^2)}{p(E^2-p_3^2)}. \tag{46}$$

Here, $\vec{p}$ is to be evaluated at the wave-packet peak value of $\vec{p}_0$. For total reflection to occur, the damping factor κ must be real. This requires that $p_3/E \ll 1$ for low to moderate potentials ($V_0 \ll m$). Consequently, the preceding equations may be simplified by neglecting quantities of the order p_3/E and V_0/E.

The first term in Eq. (46) represents that part of the longitudinal shift (dependent on the potential) that is common to both eigenpolarization states. It appears to approach infinity as the critical angle for total reflection is approached ($\kappa \to 0$). However, the stationary-phase approximation employed, which extracts mean values at the peak momentum, restricts the validity of this form to values of κ greater than the momentum spread of the wave packet. This is consistent with the assumption that all components of the wave packet undergo total reflection.

The spatial longitudinal splitting of the two single-surface polarization eigenstates, $D_l(+\hat{s}_e) - D_l(-\hat{s}_e)$, is independent of the potential and agrees completely with the expression obtained by Miller and Ashby[5] in their single-surface treatment of electrons reflecting from an infinite ramp potential. This splitting is at most of the order of a Compton wavelength. The fact that the single-surface treatment gives no transverse shift for the polarization eigenstates again agrees with Miller and Ashby. However, one must not infer from a phase-cumulation argument that a transverse shift cannot occur for a process involving a series of total reflections. As we have shown in an earlier paper,[6] the unsplit polarization eigenstates for a two-surface reflection process may undergo a transverse shift which is additive in a multireflection process.

IV. ANALYSIS BASED ON THE EXPECTATION VALUE OF A POSITION OPERATOR

In the preceding section, we have obtained the single-surface shifts by means of a phase-shift analysis that has employed a localization form-invariance argument coupled with the method of stationary phase. However, in quantum theory it would be natural to obtain the shifts by calculating the expectation value of a position operator using the incident wave packet and compare this to a similar calculation using the reflected wave packet. In this way a simple straightforward determination of the shifts can be found. Indeed if this approach is used in the nonrelativistic theory, the calculated expressions for the shifts would agree exactly with those obtained from a phase-shift analysis. However, in the relativistic theory the situation is not so simple. As we have seen in Sec. III, the complexity of the four-component wave function, which has relative phases among its components, requires that great care must be taken in a phase-shift analysis to identify the relevant phases and polarization states. Moreover, a calculation of the shifts by means of expectation values raises two problems not encountered in the nonrelativistic theory. First, instead of a unique position operator, there are a number of operators[8] to describe the position of a physical system in relativistic theory. Secondly, for an expectation-value calculation one must identify those initial polarized wave-packet states of the system that are not spatially split by the reflection process. Otherwise, an expectation-value calculation will yield a mean shift of the two polarization components that individually are shifted by different amounts. We shall consider these problems in our expectation-value calculation.

First, we shall develop the general formulation of an expectation-value calculation of the shifts. For this purpose, we begin by examining the kinematic aspects of the displacement of the outgoing motion relative to the incoming motion. The asymptotic trajectory of the center of the wave packet for the incident particle is

$$\vec{x}^I = \vec{v}^I t + \vec{x}_0^I, \tag{47}$$

while for the reflected particle the asymptotic trajectory is

$$\vec{x}^R = \vec{v}^R t + \vec{x}_0^R. \tag{48}$$

If the electron upon reflection had not undergone spatial displacement, then the trajectory of the reflected particle would be the same as Eq. (47) except for the change in sign of the $\hat{x}_3$ component of the velocity. This geometrically reflected wave packet would have a trajectory given by

$$\vec{x}^G = \vec{x}^I - 2(\vec{x}^I \cdot \hat{x}_3)\hat{x}_3. \tag{49}$$

The displacements are obtained from the difference between the physically and geometrically reflected waves. Thus, the time delay is

$$\tau = -\left(\frac{E}{p^2}\right)\vec{p}'\cdot(\vec{x}^R - \vec{x}^G), \tag{50}$$

the transverse component is

$$D_t = \rho^{-1}(\vec{p}'\times\hat{x}_3)\cdot(\vec{x}^R - \vec{x}^G), \tag{51}$$

and the longitudinal component is

$$D_l = (p\rho)^{-1}(\vec{p}'\times\hat{x}_3)\times\vec{p}'\cdot(\vec{x}^R - \vec{x}^G). \tag{52}$$

The trajectories $\vec{x}^R$ and $\vec{x}^I$ may be obtained by calculating expectation values of the appropriate position operator using the incident and reflected wave packets given in Sec. III. Several of the position operators discussed in the literature will be considered.

The Newton-Wigner position operator in the Dirac representation is given by

$$\vec{x}_{NW} = \vec{x} + \frac{i}{2E}\beta\vec{\alpha} - \frac{1}{2E(E+m)}\vec{\sigma}\times\vec{p} - \frac{1}{2E^2(E+m)}i\beta(\vec{\alpha}\cdot\vec{p})\vec{p}. \tag{53}$$

This was obtained from an analysis of localized states for elementary systems[9] so it appears especially suitable for calculating a shift in localization of an electron undergoing total reflection. In the FW representation this operator is transformed to $\vec{x}$, so it is convenient to calculate the expectation values in the FW representation.

For the physically reflected trajectory, we employ the reflected wave packet [Eq. (29)], taking the spinor factor in the FW representation [Eq. (24)]. It follows that

$$\langle\vec{x}^R\rangle = \int d^3P f^*(\vec{P}-\vec{p}_0,\hat{S})\,i\vec{\nabla}_{\vec{p}}\,f(\vec{P}-\vec{p}_0,\hat{S}) + \int d^3P|f(\vec{P}-\vec{p}_0,\hat{S})|^2\{\vec{\nabla}_{\vec{p}}[Et+\delta(p)+\chi(\vec{p},\hat{s})+\Delta(-\theta_0,\hat{s})]+\Phi^\dagger(\hat{s}')\,i\vec{\nabla}_{\vec{p}}\,\Phi(\hat{s}')\}. \tag{54}$$

Using the incident wave-packet [Eq. (27)], the geometrically reflected trajectory is obtained from Eq. (49) by taking the expectation value. This yields the result

$$\langle\vec{x}^G\rangle = \int d^3P f^*(\vec{P}-\vec{p}_0,\hat{S})\,i\vec{\nabla}_{\vec{p}}\,f(\vec{P}-\vec{p}_0,\hat{S}) + \int d^3P|f(\vec{P}-\vec{p}_0,\hat{S})|^2\{\vec{\nabla}_{\vec{p}}[Et+\Delta(-\theta_0,\hat{s})]+\Phi^\dagger(\hat{s})\,i\vec{\nabla}_{\vec{p}}\,\Phi(\hat{s})\}. \tag{55}$$

Now by direct calculation

$$\Phi^\dagger(\hat{s})\,i\vec{\nabla}_{\vec{p}}\,\Phi(\hat{s}) = \tfrac{1}{2}\cos\theta_s\,\vec{\nabla}_{\vec{p}}\,\phi_s; \tag{56}$$

a similar expression is obtained for the $\hat{s}'$ states. Substituting these expressions together with the derivatives of $\delta(\vec{p})$ and $\chi(\vec{p},\hat{s})$ into Eqs. (54) and (55), we obtain an integral form for the expectation values. These integrals may be evaluated by considering the wave packet sharply peaked at $\vec{p}_0$, so that

$$g(\vec{p}_0) = \frac{\int d^3P\, g(\vec{p}) f^*(\vec{P}-\vec{p}_0,\hat{S}) f(\vec{P}-\vec{p}_0,\hat{S})}{\int d^3P|f(\vec{P}-\vec{p}_0,\hat{S})|^2}. \tag{57}$$

When these values are substituted into Eqs. (50)–(52) we obtain

$$\tau = \frac{p_3[m^2(E-V_0)+E(E^2-p_3^2)]}{\kappa(E^2-p_3^2)p^2} + \frac{\rho p_3 m}{(E^2-p_3^2)p^2}(\hat{s}\cdot\hat{s}_t), \tag{58}$$

$$D_t = \frac{p_3}{(E+m)^2(E^2-p_3^2)} \times[\rho p_3(\hat{s}\cdot\hat{x}_3)+(E^2-p_3^2+mE)(\hat{s}\cdot\hat{x}_3\times\hat{s}_t)], \tag{59}$$

and

$$D_l = \frac{\rho[2E^2-p_3^2-EV_0]}{\kappa p(E^2-p_3^2)} - \frac{(Em+p_3^2-E^2)}{p(E^2-p_3^2)}(\hat{s}\cdot\hat{s}_t), \tag{60}$$

where we have relabeled $\vec{p}_0$ by $\vec{p}$. These expressions for the shifts and time delay are mean quantities for an arbitrary incident polarization direction $\hat{s}$. In order to find those initial polarization states that do not become spatially split by a single-surface reflection process, we must invoke the form-invariance localization argument of Sec. III which yields the single-surface eigenpolarization states $\pm\hat{s}_e$ given in Eq. (34). We note that when evaluated at $\vec{p}=\vec{p}_0$, $\hat{s}_e$ becomes simply $-\hat{s}_t$. Consequently for the unsplit single-surface eigenpolarization states, Eqs. (58)–(60) are the same as Eqs. (44)–(46) given by the phase-shift analysis method.

The appearance of a mean transverse shift for an arbitrary state of polarization is due to the interference between the two split components (corresponding to the eigenpolarization states) of the incident beam. Similarly, the mean longitudinal shift and the mean time delay have contributions from these interference terms.

To illustrate how the expectation-value calculation of the shifts depends on which position operator is used, we will do a similar calculation using the operator $\vec{x}$ in the Dirac representation. The transform of this operator to the FW representation is given by

$$\vec{x} - \frac{\vec{\sigma}\times\vec{p}}{2E(E+m)}, \tag{61}$$

where all odd-operator terms have been dropped since they do not enter the expectation-value calculations. When acting between positive-energy states this operator is the same as the center-of-mass position operator.[10,11] With reference to the results obtained from the Newton-Wigner position operator, the additional contribution to the transverse shift is m/E times the expression given in Eq. (59) and the additional contribution to the longitudinal shift is

$$-\frac{p}{E(E+m)}(\hat{s}\cdot\hat{s}_t). \tag{62}$$

There are no additional contributions to the time delay. The additional terms are at most of the order of the Compton wavelength.

Another position operator which has been extensively used in the literature is the center-of-inertia operator.[11,12] In the FW representation it assumes the form

$$\vec{x} + \frac{\vec{\sigma}\times\vec{p}}{2m(E+m)}. \tag{63}$$

The additional contribution to the shifts for the center-of-inertia operator can be obtained from the results given for center-of-mass operator by changing the sign of the terms and replacing E in the denominator by m. Thus for all polarization directions there is no transverse shift.

The results presented above for these other position operators are given for purposes of comparison to those obtained for the Newton-Wigner position operator. It is the set of results obtained for the Newton-Wigner position operator which agrees with the phase-shift method of analysis given in Sec. III.

V. CURRENT-FLUX METHOD OF CALCULATING DISPLACEMENTS

Another method of calculating the displacements, used extensively in the literature[3] on the Goos-Hänchen effect for light, is based on conservation of current. Using the optical Fresnel relations for total reflection of an incident plane wave of arbitrary polarization, it is easy to show that in the evanescent wave there exists a nonzero time-averaged Poynting vector parallel to the reflecting surface. From this one can infer that energy is transferred from the incident light beam to the medium of lower index of refraction, flows along that side, and then this energy subsequently reemerges in the reflected wave. Thus, the beam will be spatially translated. In the steady-state situation, the principle of conservation of energy is used to establish the quantitative expression for the shift. Using the Schrödinger equation, Renard has applied this method to find the shifts for a particle beam. In a quantum-mechanical treatment of this type, the current-flux approach may be equivalently considered as a conservation of probability (or particles) method. In this section, we shall use this approach in a straightforward way to calculate the shifts for a Dirac electron undergoing total reflection.

As is customary in the application of the current-flux method we will employ a plane wave to represent the central region of the beam. Utilizing current-flux conservation we see from Fig. 1 that the flux of incident current through a strip of the boundary surface of unit width and of length D (the shift) aligned in the direction of the evanescent current should be equal to the flux of the evanescent current through the semi-infinite strip of that width extending from $x_3 = 0$ to $x_3 = \infty$. Thus,

$$\vec{D}J_3(0) = \int_0^\infty \vec{J}\,dx_3, \tag{64}$$

where $\vec{D}$ is taken to be the displacement (shift) on the boundary plane of the reflected plane wave relative to the incident plane wave. $\vec{J}$ is the evanescent current, and $J_3(0)$ is the x_3 component of incident current evaluated at the boundary surface. Substituting Eqs. (20) and (21) into Eq. (64), we obtain the results

$$D_t = \frac{p_3}{V_0(E+m)(E^2-p_3^2)} \times [\rho p_3(\hat{s}\cdot\hat{x}_3) + (E^2-p_3^2+mE)(\hat{s}\cdot\hat{x}_3\times\hat{s}_t)], \tag{65}$$

and

$$D_L = \frac{\rho p_3(E-V_0)}{V_0\kappa(E^2-p_3^2)} - \frac{mp_3}{V_0(E^2-p_3^2)}(\hat{s}\cdot\hat{s}_t). \tag{66}$$

The longitudinal shift D_L, measured in the plane of the boundary surface, is related to the shift D_t defined in Eq. (40) by $D_t = (p_3/p)D_L$.

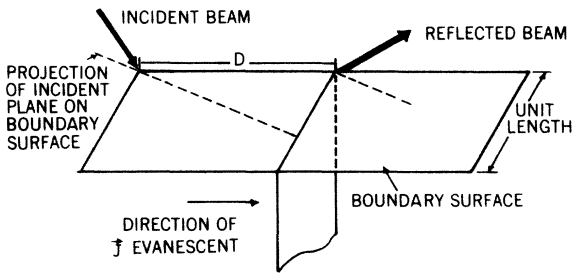

FIG. 1. Geometric configuration utilized in calculation of shifts based on conservation of current flux.

The polarization-dependent terms of Eqs. (65) and (66) exhibit an inverse V_0 dependence. In contrast, the polarization-dependent terms obtained from either the phase-shift analysis or from an expectation-value calculation of a position operator are independent of the potential. Moreover, the phase-shift analysis of Sec. III or any of the expectation-value calculations of Sec. IV give the same expression for the polarization-independent term of the longitudinal shift, namely the first term of Eq. (46). The current-flux argument produces a different result for this term [cf. Eq. (66)]. However, these two expressions for the polarization-independent part of the longitudinal shift agree near the critical angle ($\kappa \to 0$). This common limit follows from the relation

$$(2E^2 - p_3^2 - EV_0) = V_0^{-1}[(E-V_0)p_3^2 + E\kappa^2]\,. \tag{67}$$

There is no direct method of calculating a time delay using the current-flux method. An indirect approach involves the estimation of the time t_L for the evanescent current to flow the shift distance. This time is

$$t_L = (D_t^2 + D_L^2)^{1/2}/v_{\text{avg}}\ , \tag{68}$$

which depends on a knowledge of the average speed of the evanescent current parallel to the surface. If this speed were known, the time t_L could be related to the time delay τ previously defined via the expression

$$\vec{x}^R = \vec{x}^G + D_t\,\hat{s}_t \times \vec{p}' + D_t\,\hat{s}_t - \tau(\vec{p}'/E)\,, \tag{69}$$

by rewriting this as

$$\vec{x}^R = \vec{x}^G + D_L(\hat{x}_3 \times \hat{s}_t) + D_t\,\hat{s}_t - \left(\tau + \frac{ED_L}{p}\right)\vec{p}'/E. \tag{70}$$

Consequently, it follows that

$$\tau = t_L - E\rho D_t/(pp_3)\,. \tag{71}$$

However, there is no simple expression, e.g., ρ/E, which can be used for the average velocity. Indeed, if one uses the results for the shifts and time delay of the eigenpolarization states given by the phase-shift method, one obtains a complicated polarization-dependent expression for v_{avg}. This expression reduces to ρ/E only near the critical angle.

VI. REMARKS

The spatial displacements for a totally reflected electron have been calculated in a number of ways in Secs. III–V. Although all of the methods give small polarization-dependent terms and the polarization-independent terms approach the same limit near the critical angle, the functional forms given by the various approaches are in disagreement.

The phase-shift analysis and the expectation-value calculation using the Newton-Wigner position operator yield the same set of results for the eigenpolarization states. Although other position operators give different results, it is the Newton-Wigner position operator which best characterizes the properties of localized states. Since the spatial displacements pertain to the localization properties of the system, it appears reasonable to employ the Newton-Wigner operator.

The symmetry of the problem implies rotational invariance about the $\hat{x}_3$ axis. Consequently, the third component of the total angular momentum is conserved. We may write this requirement in the form

$$\begin{aligned}\langle S_3\rangle^I &= \langle S_3\rangle^R + (\vec{D}\times\vec{p})_3 \\ &= \langle S_3\rangle^R + \rho D_t\ .\end{aligned} \tag{72}$$

The appropriate spin operators which are to be used in the above equation will depend on which position operator is used in evaluating the displacements. For the Newton-Wigner position operator the spin operator is just $\frac{1}{2}\vec{\sigma}$ in the FW representation. When the expectation value of $\frac{1}{2}\vec{\sigma}_3$ is calculated for the incident and reflected FW states, Eq. (72) is satisfied if the expression for D_t given by Eq. (59) is used.

In order to see whether the expression for D_t obtained from the current-flux method is consistent with conservation of the third component of angular momentum, a position operator that yields this D_t and an associated spin operator must be determined. As we have seen, none of the position operators examined in this paper produce a transverse shift equal to that obtained by the current-flux method. Furthermore, since that polarization-dependent transverse shift is also potential-dependent, a suitable position operator must contain terms that produce this dependence, e.g., terms of the type $(\vec{x}\cdot\vec{F})\,(\vec{\sigma}\cdot\vec{G})$ or terms quadratic in $\vec{x}$. None of the usual operators that in some sense characterize the position of a system have such terms. Thus, it appears that the displacements given by the current-flux method violate the conservation of the third component of angular momentum.

The failure of the current-flux method can be traced to the use of plane waves in evaluating the currents. If a localized wave-packet description were incorporated into the current, then one should be able to calculate the displacements by finding how the evanescent-current flux through the semi-infinite plane normal to the boundary falls off as a function of distance from the center of the impact of the incident wave packet. However, if one attempts such a calculation, one is led to a multiple integral for that flux which cannot be reduced to a closed-form expression.

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Derivation of gauge invariance from high-energy unitarity bounds on the S matrix*

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A systematic search is made for all renormalizable theories of heavy vector bosons. It is argued that in any renormalizable Lagrangian theory high-energy unitarity bounds should not be violated in perturbation theory (apart from logarithmic factors in the energy). This leads to the specific requirement of "tree unitarity": the N-particle S-matrix elements *in the tree approximation* must grow no more rapidly than E^{4-N} in the limit of high energy (E) at fixed, nonzero angles (i.e., at angles such that all invariants $p_i \cdot p_j$, $i \neq j$, grow like E^2). We have imposed this tree-unitarity criterion on the most general scalar, spinor, and vector Lagrangian with terms of mass dimension less than or equal to four; a certain class of nonpolynomial Lagrangians is also considered. It is proved that any such theory is tree-unitary if and only if it is equivalent under a point transformation to a spontaneously broken gauge theory, possibly modified by the addition of mass terms for vectors associated with invariant Abelian subgroups. Our result suggests that gauge theories are the only renormalizable theories of massive vector particles and that the existence of Lie groups of internal symmetries in particle physics can be traced to the requirement of renormalizability.

I. INTRODUCTION

The only systems of heavy vector bosons which are known to be renormalizable are spontaneously broken gauge theories[1] (SBGT's) and "conserved current" models. In an SBGT the field variables can always be chosen so that the Lagrangian is locally gauge-invariant. The vector bosons acquire mass through the mechanism of spontaneous symmetry breaking. Massless vector bosons have conserved source currents. On the other hand, "conserved current" models always contain at least one massive vector boson whose source current is conserved. Massive quantum electrodynamics (QED) is the simplest system of this type. The general prescription for constructing conserved-current models can be stated as follows: (1) Begin with a Lagrangian which is invariant under a nonsemisimple group of local gauge transformations (i.e., a group of transformations containing an invariant Abelian subgroup). (2) Arrange for spontaneous symmetry breaking (if any) such that the vacuum expectation values of the scalar fields are invariant under at least one invariant (single-parameter) Abelian subgroup (thus, at this stage the corresponding Abelian vector is massless and coupled to a conserved current). (3) Add an arbitrary mass term for the same Abelian vector. Notice that the Lagrangian is invariant under the entire group of global gauge transformations and under the semisimple subgroup of local gauge transformations.

Most massive vector Lagrangians are not renormalizable because the $k_\mu k_\nu$ term in the vector propagator induces "bad" high-energy behavior in the scattering amplitudes. Conserved-current and SBGT models are renormalizable because this "bad" high-energy behavior is vitiated by the symmetry of the vector couplings which multiply the "bad" $k_\mu k_\nu$ factors. For example, in conserved-