# Complete Keldysh theory and its limiting cases

H. R. Reiss
*Department of Physics, The American University, Washington, D.C. 20016*
(Received 5 July 1989)

An investigation of the foundations of strong-field theories of the Keldysh type is undertaken. It is found first that the Volkov solution, upon which the Keldysh approximation depends, exists unambiguously only in the relativistic case. Accordingly, a fully relativistic theory of atomic photoionization is formulated from first principles. A strong-field approximation (SFA) is expressed, based only on the proposition that the photoionizing field dominates the atomic potential in the final state. The nonrelativistic limit of the SFA gives exactly one of the known Keldysh-type theories, but the original Keldysh theory itself is found to neglect some fraction of the strong-field effects. It is shown on a variety of grounds that $\mathbf{A}^2$ terms must be fully retained in Keldysh-type theories. Important in this matter are the proper application of asymptotic conditions, the interchangeability of $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms, and the consistent reduction to the nonrelativistic limit.

## I. INTRODUCTION

Atomic photoionization in strong fields is treated from first principles. The theory developed here is based solely on the dominance of the applied field over the atomic potential in the final state in photoionization. It is referred to as the strong-field approximation (SFA). The formal structure is suggestive of the well-known Keldysh[1] approximation, in which the transition amplitude is approximated by treating the effect of the atomic binding potential on the detached electron as an influence small with respect to external field effects. The full development given here shows, however, that some field-dependent terms are lost in the original Keldysh formulation because they cross-couple to atomic potential terms. This is not necessary, and the SFA given here does not have that limitation. Upon reduction to the nonrelativistic limit, the SFA reduces exactly to one[2] of the published versions of a Keldysh-like theory.

The physical problem is formulated from an $S$-matrix approach, since this permits a clear statement of the all-important boundary conditions, and it lends itself to both nonperturbative and perturbative methods. It is found that one is led to the Volkov solution,[3] an exact solution for an electron in a packet of unidirectional electromagnetic plane waves. It is important to observe that there is no such thing as a nonrelativistic Volkov solution despite the reliance formerly placed on such putative solutions. The point is that a free-particle solution must be valid over many wavelengths of the field or it is not a free-particle solution at all. The dipole approximation can be invoked only when there is justification for it, as when a true Volkov solution is incorporated into a transition matrix element with a bound-state solution, which effectively limits the range of the spatial coordinate. Without the dipole approximation, the only solutions for a free particle in a plane-wave field are relativistic, and one must enter the transition matrix element with such a solution.

To be consonant with the introduction of relativistic Volkov solutions, it is necessary for the entire formalism to be relativistic. Furthermore, it is known that sufficiently strong fields in themselves will induce relativistic motions in free electrons. A theory which undertakes to be a truly strong-field theory must then be relativistic in its foundations. The theory formulated here is a theory of a scalar (or spinless) electron, based on solutions of the Klein-Gordon equation. This is done because reduction to the nonrelativistic limit can be effected quite simply and generally. A Dirac theory, fully inclusive of spin effects, can also be developed.[4,5]

The present investigation provides a valuable framework for the clear examination of an issue which is central for strong-field photoionization, but which has not been addressed definitively. That issue is the proper treatment of the $\mathbf{A}^2$ term. When the dipole approximation is introduced, this term appears in the Volkov solution as a purely time-dependent phase factor, and so there is a temptation to remove it by a contact transformation.[6–8] That is shown from three distinct sets of reasons not to be a proper procedure. This matter is given prominence here because an examination of this issue serves to clarify the reasons underlying persistent misinterpretations of the structure of Keldysh-like theories, and it also serves to emphasize some of the distinctions between a field-dominated theory such as the SFA or the Keldysh approximation, and the more familiar atomic-potential-dominated theories. Each of the three bases on which it is shown that $\mathbf{A}^2$ must be retained is "robust" in itself, and is sufficient cause to retain that all-important contribution. Taken together, these three arguments are very powerful.

The first basis for recognizing the need for full retention of the $\mathbf{A}^2$ term comes directly from the $S$-matrix formalism, which allows one to be very clear about the application of proper boundary conditions. The standard boundary conditions in the $S$-matrix formalism are designed to recognize that measurements to assess the

 

effects of the field are done in the asymptotic region, where the field causing the photoionization is not itself present. Hence the $\underline{S}$ matrix contains both a fully interacting state and a "reference state" which has no field interaction at all. Removal of the $\mathbf{A}^2$ term from the interacting state corresponds to a shift in the energy of that state which can be substantial. Unless the reference state is also so shifted (which cancels the contact transformation) there will be a wholly unphysical alteration in the energy of the system introduced thereby.

A second view of the $\mathbf{A}^2$ problem comes from the relativistic formulation of the SFA. This negates any possibility of the contact transformation generally invoked to manipulate the $\mathbf{A}^2$ term, since it is now dependent on the position coordinate $\mathbf{r}$. When the nonrelativistic, dipole-approximation limit is taken, very large contributions of $\mathbf{A}^2$ remain, whose arbitrary removal radically alters physical predictions. The form of the result before taking limits must be correct when any seeming ambiguity can arise. Hence $\mathbf{A}^2$ removal cannot be correct.

A further reason to preserve fully the $\mathbf{A}^2$ term at every stage of the calculation comes from basic field-interaction considerations. In a multiphoton process, there is no true distinction between $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ contributions. At any order above the first, there are transformations which interchange them. The phase coupling of the $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms is vitally important at any order above the first, and this is shown below to be sustained even in the weak-field limit. In brief, one cannot properly manipulate the $\mathbf{A}^2$ term by itself in a multiphoton problem.

Finally, it must be noted that most arguments for removal of $\mathbf{A}^2$ rely on setting $\mathbf{A}(\mathbf{r},t)\rightarrow\mathbf{A}(t)$ at the outset of the demonstration. That is rather like trying to explore the limit as $x\rightarrow 0$ of $(\sin x)/x$, or $(\sin x)^2/x$, or $(\sin x)/x^2$ by starting with $x=0$. It is important to apply the limit properly when exploring the electric dipole approximation (EDA).

The need for care in formulating the problem and in applying limiting procedures can be appreciated by noting some of the orders of magnitude associated with basic field-interaction terms. As a practical example, consider the $CO_2$ laser environment (10.6 $\mu$m) at $10^{15}$ W/cm$^2$. The $e^2\mathbf{A}^2/2mc^2$ interaction term has a magnitude of about 10 keV, as does the $e\,\mathbf{A}\cdot\mathbf{p}/2mc$ term when evaluated for a momentum corresponding to the peak of the above-threshold ionization (ATI) spectrum for a circularly polarized field. These field-interaction energies are to be contrasted to atomic binding energies, which are a thousand times smaller.

The SFA is a completely formulated theory starting from exact expressions. In apparent conflict with this picture of a Keldysh-type theory as a strong-field approximation, well founded on first principles, some investigators have concluded that the theory is internally inconsistent[6] or even that it is a weak-field theory.[7–9] A feature common to these researchers is that they remove the $\mathbf{A}^2$ term from the theory. The inconsistencies they find are the inconsistencies bound to flow from this step. Other investigators have undertaken to compare[9,10] a one-dimensional version of Keldysh-style theories with one-dimensional numerical models of atomic photoionization, and find that Keldysh methods fare poorly. A "one-dimensional Keldysh-style theory" would require use of a one-dimensional Volkov solution, which does not exist. "One-dimensional Keldysh-style" calculations differ radically (and unphysically) from three-dimensional calculations of the very same processes by a true Keldysh-style theory.[11]

It is well to emphasize again that the theory to be developed here is a strong-field theory which differs in many respects from conventional atomic theory. These differences can take the form of distinct physical interpretations of the same phenomenon, or they can be important quantitative differences. As one illustration of the former, the phenomenon of peak suppression in above-threshold ionization is sometimes described in atomic theory in terms of field-induced atomic energy level shifts. In a Keldysh-style theory this same phenomenon arises as the need to supply to the detached photoelectron its minimal energy of interaction with the plane-wave field.[2,12]

The organization of this paper is that Sec. II is concerned with wave equations. First the free electron in a plane-wave field is considered (Volkov solution), and then the complete situation is addressed, with the atomic potential simultaneously present. Section III is devoted to the development of the transition amplitude. It is first expressed exactly by way of an $\underline{S}$-matrix theory. It is shown how perturbation theory arises from this formalism, and then the SFA is developed. The nonrelativistic limit of the SFA is found in Sec. IV. Section V is devoted to an examination of the $\mathbf{A}^2$ problem from the three points of view summarized above. Appendix A is dedicated to a derivation of the Klein-Gordon $\underline{S}$ matrix. Appendix B gives a simple nonperturbative derivation of the Fermi "golden rule" starting from the $\underline{S}$-matrix formulation, and applied to problems exhibiting the Floquet property.

## II. WAVE FUNCTIONS

### A. Volkov solution

The Volkov solution is an exact solution for a free charged particle in an electromagnetic plane wave. Historically, this was first written down[3] for a relativistic spinor electron obeying the Dirac equation, but a minor modification of this result produces a solution for a relativistic scalar charged particle obeying the Klein-Gordon equation. Keldysh-type theories, however, have been based[1,2] on a putative solution to the nonrelativistic Schrödinger equation with the field rendered in the EDA

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t)=\frac{1}{2m}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(t)\right]^2\Psi(\mathbf{r},t)\,, \tag{2.1}$$

where $\mathbf{p}$ is the canonical momentum operator and $\mathbf{A}$ is the vector potential describing the field. The essential point is that $\Psi$ satisfying Eq. (2.1) is *not* a Volkov solution. The reason is that a Volkov solution must describe a free particle. It must therefore be applicable over many wavelengths. It is not correct to restrict the motion to a small fraction of a wavelength in the original equation of

motion. However, if one generalizes Eq. (2.1) from $\mathbf{A}(t)$ to $\mathbf{A}(\omega t-\mathbf{k}\cdot\mathbf{r})$, then there is no known solution to Eq. (2.1) so generalized. To find an unambiguous free-particle solution, it is necessary to employ the only true Volkov solutions, which are relativistic. Reduction to the electric dipole approximation and the nonrelativistic limit cannot be done directly in the Volkov solution, since there is no *ab initio* justification for doing that. That justification comes about only when the Volkov solution is folded together in a transition matrix element with a bound-state solution for the electron. The transition matrix element must be entered with a proper solution to the equation of motion.

The Volkov solution to be employed will be for a scalar particle, since it is much more transparent to see how the EDA and nonrelativistic limits come about in that case than it is when working with the spinor Dirac solution. Units with $\hbar=1$ and $c=1$ will now be employed, and the relativistic conventions and notation of Bjorken and Drell[13] will be adopted. In brief, these conventions are that four-vectors bear Greek indices that range from 0 to 3, and a time-favoring real metric is used. An inner product is given by, for example, $p\cdot x\equiv p_\mu x^\mu=p^\mu x_\mu=Et-\mathbf{p}\cdot\mathbf{r}$; where the energy $E$ and three-momentum $\mathbf{p}$ are the time and space parts of the four-momentum $p^\mu$, and $t$ and $\mathbf{r}$ are time and space parts of $x^\mu$. The Klein-Gordon equation in the presence of a field described by the four-vector potential $A^\mu$ is

$$\{[i\partial_\mu-eA_\mu(x)][i\partial^\mu-eA^\mu(x)]-m^2\}\Psi(x)=0\ , \tag{2.2}$$

where functional dependence on $x$ refers to the four-vector $x^\mu$. Equation (2.2) may be rewritten with interaction terms separated as

$$(\partial^\mu\partial_\mu+m^2)\Psi(x)=-\mathcal{V}_{\rm KG}(x)\Psi(x)\ , \tag{2.3}$$

where $\mathcal{V}_{\rm KG}(x)$ is defined by

$$\mathcal{V}_{\rm KG}=ie(\partial_\mu A^\mu+A^\mu\partial_\mu)-e^2A_\mu A^\mu\ , \tag{2.4}$$

in terms of the abbreviated notation $\partial^\mu\equiv\partial/\partial x_\mu$ and $\partial_\mu\equiv\partial/\partial x^\mu$.

When the vector potential $A^\mu$ represents a packet of electromagnetic plane waves all propagating in a single direction, an exact solution of Eq. (2.2) is given by either

$$\Psi^{(+)}=(2EV)^{-1/2}\exp\left[-ip\cdot x-i\int_{-\infty}^{k\cdot x}d(k\cdot x')\left[\frac{eA\cdot p}{p\cdot k}-\frac{e^2A\cdot A}{2p\cdot k}\right]_{(k\cdot x')}\right] \tag{2.5}$$

or

$$\Psi^{(-)}=(2EV)^{-1/2}\exp\left[-ip\cdot x+i\int_{k\cdot x}^{\infty}d(k\cdot x')\left[\frac{eA\cdot p}{p\cdot k}-\frac{e^2A\cdot A}{2p\cdot k}\right]_{(k\cdot x')}\right]\ , \tag{2.6}$$

satisfying the boundary conditions

$$\lim_{k\cdot x\to-\infty}\Psi^{(+)}(x)=\Phi(x),\quad \lim_{k\cdot x\to+\infty}\Psi^{(-)}(x)=\Phi(x)\ . \tag{2.7}$$

The function $\Phi(x)$ in Eq. (2.7) is the noninteracting solution which satisfies

$$(\partial^\mu\partial_\mu+m^2)\Phi(x)=0\ . \tag{2.8}$$

The solution given by Eq. (2.5) or by (2.6) is a Klein-Gordon Volkov solution.

### B. Plane-wave field plus binding potential

To write the Klein-Gordon equation for a combined plane-wave field and static binding potential, Eq. (2.2) can be employed with the replacement

$$A^\mu\to A^\mu+g^{\mu0}V(\mathbf{r})\ , \tag{2.9}$$

where $g^{\mu\nu}$ is the metric tensor of special relativity, and where the continued appearance of $A^\mu$ on the right-hand side is meant to represent the plane-wave electromagnetic field, as before. That is, the right-hand side of Eq. (2.9) is a sum of transverse and longitudinal terms. When substituted into Eq. (2.2), (2.9) gives uncoupled transverse and longitudinal interaction terms plus a cross coupling given by $2VeA^0$. Equation (2.3) is then replaced by

$$(\partial^\mu\partial_\mu+m^2)\Psi(x)=-(\mathcal{V}^F+\mathcal{V}^A+2VeA^0)\Psi(x)\ , \tag{2.10}$$

where $\mathcal{V}^F$ is the field-interaction operator [as in Eq. (2.4)] and $\mathcal{V}^A$ is the atomic interaction operator, given by

$$\mathcal{V}^F=i\partial_\mu eA^\mu+eA^\mu i\partial_\mu-e^2A^\mu A_\mu\ , \tag{2.11}$$

$$\mathcal{V}^A=i\partial_0V+Vi\partial_0-V^2\ . \tag{2.12}$$

The last term on the right-hand side in Eq. (2.10) represents a coupling between the external field and the atomic potential which is an impediment to straightforward application of a strong-field approximation. The radiation gauge (or Coulomb gauge) is explicitly designed to decouple longitudinal and transverse fields. In this

gauge $A^0$ vanishes, and the cross-coupling term along with it. Apart from later remarks about the cross-coupling term in the Keldysh approximation, the radiation gauge will be adopted from here on.

Because of the decoupling of the field and atomic interactions, the equation of motion for the combined interactions can be written either as

$$[(i\partial_\mu - eA_\mu)(i\partial^\mu - eA^\mu) - m^2 - \mathcal{V}^A]\Psi(x) = 0 , \tag{2.13}$$

or as

$$[(i\partial_\mu - Vg_{\mu 0})(i\partial^\mu - Vg^{\mu 0}) - m^2 - \mathcal{V}^F]\Psi(x) = 0 . \tag{2.14}$$

It is Eq. (2.13) which provides the form relevant here, since it leads to the integral equation solution

$$\Psi(x) = \Psi^F(x) + \int d^4x' G^F(x,x')\mathcal{V}^A(x')\Psi(x') , \tag{2.15}$$

in terms of the Volkov solution (here designated by $\Psi^F$) and the Volkov Green's function $G^F(x,x')$. This Volkov Green's function satisfies the equation

$$\{[i\partial_\mu - eA_\mu(x)][i\partial^\mu - eA^\mu(x)] - m^2\}G^F(x,x') = \delta^4(x - x') . \tag{2.16}$$

The state $\Psi$ in (2.15) is the complete solution for Eq. (2.10), (2.13), or (2.14). The integral equation (2.15) can be solved by iteration to yield the successive approximations

$$\Psi^{(0)}(x) = \Psi^F(x) , \tag{2.17}$$

$$\Psi^{(1)}(x) = \Psi^F(x) + \int d^4x' G^F(x,x')\mathcal{V}^A(x')\Psi^F(x') , \tag{2.18}$$

$$\Psi^{(2)}(x) = \Psi^F(x) + \int d^4x' G^F(x,x')\mathcal{V}^A(x')\Psi^F(x') + \int d^4x' \int d^4x'' G^F(x,x')\mathcal{V}^A(x')G^F(x',x'') \times \mathcal{V}^A(x'')\Psi^F(x'') , \tag{2.19}$$

and so on. Equations (2.17)–(2.19) and the logical continuation thereof represent an expansion of the complete wave function in powers of the atomic potential $\mathcal{V}^A$. This is in contrast to the more usual procedure which underlies ordinary perturbation theory, in which the starting point is Eq. (2.14) and the expansion is in powers of $\mathcal{V}^F$, due to the applied plane-wave field.

The procedure introduced above is the one which is appropriate under circumstances in which it is expected that the applied electromagnetic field will be dominant in magnitude over the atomic field. An illustration of this situation is provided by the explicit example cited earlier ($CO_2$ laser environment at $10^{15}$ W/cm$^2$) in which the expectation value of $\mathcal{V}^F/2m$ is about 10 keV, whereas that of $\mathcal{V}^A/2m$ is only about 10 eV.

## III. TRANSITION AMPLITUDE

### A. Exact $\underline{S}$ matrix

The exact $\underline{S}$ matrix can be written as

$$S_{fi} = \lim_{t\to+\infty}(\Phi_f, \Psi_i^{(+)}), \quad \lim_{t\to-\infty}\Psi_i^{(+)} = \Phi_i , \tag{3.1}$$

or as

$$S_{fi} = \lim_{t\to-\infty}(\Psi_f^{(-)}, \Phi_i), \quad \lim_{t\to+\infty}\Psi_f^{(-)} = \Phi_f . \tag{3.2}$$

In these expressions, $\Psi$ represents the complete physical environment with all interactions present, whereas $\Phi$ is a reference state, free of the transition-causing interaction, against which $\Psi$ is compared. That is, Eq. (3.1) corresponds to the measurement process in which the final result of the interaction causing the transition is appraised by detection of the final outcome of the experiment in a detector located outside of the interaction region. Equation (3.1) is the probability amplitude that a state initially prepared as $\Phi_i$ has been transformed into a different noninteracting state $\Phi_f$. Equation (3.2) is the time-reversed version of (3.1), and is more suitable for the development of the SFA.

The $\underline{S}$ matrices defined in Eqs. (3.1) and (3.2) can be converted[13] to finite times in a relativistically covariant way suitable for scalar particles. The procedure is given in Appendix A. The results [Eqs. (A12) and (A13)] are

$$(\underline{S} - \underline{1})_{fi} = -i\int d^4x\, \Phi_f^*\mathcal{V}^F\Psi_i^{(+)} , \tag{3.3}$$

$$(\underline{S} - \underline{1})_{fi} = -i\int d^4x\, \Psi_f^{(-)*}\mathcal{V}^F\Phi_i . \tag{3.4}$$

It is reiterated that these equations are exact as long as $\Psi$ is exact. Since an exact $\Psi$ is not normally known, an approximation must be employed. There is more than one systematic procedure for doing this.

For later discussion about the $\mathbf{A}^2$ term, it is stressed that the functions $\Phi$ in Eqs. (3.3) and (3.4) are both reference states which are *free of the transition-causing interaction* $\mathcal{V}^F$.

### B. Perturbation theory

Equation (3.4) will be made the focus of attention. The conventional approach via perturbation theory is to expand $\Psi_f$ in powers of the interaction term $\mathcal{V}^F$. The zeroth-order term in the expansion of $\Psi_f$ is just $\Phi_f$, in which case the first approximation to Eq. (3.4) is

$$(\underline{S} - \underline{1})_{fi}^{(1)PT} = -i\int d^4x\, \Phi_f^*\mathcal{V}^F\Phi_i . \tag{3.5}$$

This contains the transition-causing interaction exactly once, as the factor $\mathcal{V}^F$. In concordance with the $\underline{S}$-matrix definition requiring the reference states to be free of the transition-causing influence, the $\Phi$ states have no dependence on $\mathcal{V}^F$ at all. The next perturbative approximation beyond Eq. (3.5) will contain a single factor $\mathcal{V}^F$ in the expression for $\Psi_f$, so there will be exactly two factors of $\mathcal{V}^F$ in the $\underline{S}$ matrix, and so on. This is the well-known structure of perturbation theory.

### C. Strong-field approximation

If the physical problem is such that the interaction $\mathcal{V}^A$ is likely to be of lesser magnitude than $\mathcal{V}^F$, a rational approach is to expand $\Psi_f$ in powers of $\mathcal{V}^A$ rather than $\mathcal{V}^F$. This is the procedure detailed in Eqs. (2.17)–(2.19). The lowest-order approximation so obtained is exactly the strong-field approximation

$$(\underline{S}-\underline{1})_{fi}^{\mathrm{SFA}}=-i\int d^4x\ \Psi_f^{(-)F*}\mathcal{V}^F\Phi_i\ , \tag{3.6}$$

where $\Psi_f^{(-)F}$ is the Volkov solution explicitly stated in Eq. (2.6).

The most noteworthy feature of Eq. (3.6) is that it is certainly not a perturbation expression in $\mathcal{V}^F$. The field interaction has been completely retained everywhere that it originally appeared in the exact $\underline{S}$ matrix. Since the Volkov solution becomes a more accurate representation of the ionized electron as the dominance of $\mathcal{V}^F$ over $\mathcal{V}^A$ increases, the approximation represented in Eq. (3.6) should improve in accuracy as $\mathcal{V}^F$ grows larger. For details about higher approximations in the SFA expansion, see Refs. 2 and 4.

Another significant feature of Eq. (3.6) is that, although it arises as the leading term in an expansion of $\Psi_f$ in powers of $\mathcal{V}^A$, the SFA is not simply a lowest-order perturbation expression in $\mathcal{V}^A$. Referring back to a true first-order perturbation expression as in Eq. (3.5), it is seen that the perturbing interaction appears once only. Because $\mathcal{V}^F$ is the influence which leads to the transition, it is nowhere involved in the reference states $\Phi_f$ or $\Phi_i$. By contrast, in Eq. (3.6), $\mathcal{V}^A$ is contained exactly—that is, to all orders—in the function $\Phi_i$. The reason for this disparity in behaviors is that $\mathcal{V}^F$ is the interaction that causes the transition and $\mathcal{V}^A$ is not. They thus appear in fundamentally different roles in the $\underline{S}$ matrix since the reference states in the SFA case are fully dependent on $\mathcal{V}^A$. A practical result of this nonperturbative dependence of the SFA on $\mathcal{V}^A$ is that one can use Eq. (3.6) to explore the consequences of different initial bound states with very important qualitative and quantitative distinctions arising therefrom.

Equation (3.6) for the SFA can be effectively simplified by an integration by parts. Two of the terms in $\mathcal{V}^F$ as shown in Eq. (2.11) contain differential operators. If an integration by parts with these two terms is carried out in Eq. (3.6), and the surface terms at infinity are dropped by the standard boundary condition on $A^\mu$, then Eq. (3.6) becomes

$$(\underline{S}-\underline{1})_{fi}^{\mathrm{SFA}}=-i\int d^4x(\mathcal{V}^F\Psi_f^{(-)F})^*\Phi_i\ . \tag{3.7}$$

The relative sign between the differential terms and the $A\cdot A$ term in $\mathcal{V}^F$ is maintained after the integration by parts because of the complex conjugation of $\mathcal{V}^F$ in Eq. (3.7). The state $\Psi_f^{(-)F}$ is an eigenstate of the operator $\mathcal{V}^F$ with the consequence that Eq. (3.7) can be rewritten as

$$(\underline{S}-\underline{1})_{fi}^{\mathrm{SFA}}=-i\int d^4x\ \Psi_f^{(-)F*}(2eA\cdot p-e^2A\cdot A)\Phi_i\ , \tag{3.8}$$

where the $p^\mu$ in Eq. (3.8) is now an eigenvalue and not an operator.

Equations (3.6) and (3.8) exhibit an important property which cannot be emphasized too strongly. As demanded by the boundary conditions expressed in Eq. (3.2), $\Phi_i$ has no interaction with the external field, and so it is a simple stationary state. On the other hand, $\Psi_f^{(-)F}$ is a Volkov state which has strong-field interaction, and, as will be seen shortly, possesses a time-dependent $A^2$ term in an exponential factor which makes an important contribution in the energy conservation condition. By contrast, Eq. (3.5) from perturbation theory has no such factor at all. The two approaches can then be very different in their predictions because the $A^2$ term can be so very large. Even if perturbation theory is carried to higher orders, the $A^2$ term never appears in an exponential factor, and $A^2$ will show up only as a polynomial term which cannot make anything like the important energy difference that is introduced by the exponentiated $A^2$. The contribution of $A^2$ to the energy is thus a true intense-field effect, which does not occur in any finite order of perturbation theory.

### D. Keldysh approximation

The SFA given above is strongly suggestive of the Keldysh approximation, since it folds together in the transition amplitude the Volkov solution for the final state, the interaction Hamiltonian, and a noninteracting initial state. This appears to be the same structure as the Keldysh approximation,[1] which was written down as an ansatz on physical grounds. However, the Keldysh theory has never been derived from first principles. It differs from the above formalism in that it is written in the so-called Göppert-Mayer gauge,[14] in which the interaction Hamiltonian takes the form $-e\mathbf{E}\cdot\mathbf{r}$. That interaction is explicitly nonrelativistic in nature, since it represents the electromagnetic field by a single (scalar) component of the four-vector potential. That is clearly not adequate for a relativistic treatment, but it is possible to generalize the Göppert-Mayer gauge to the relativistic case.[15] (It is done in Ref. 15 for a monochromatic field, but it is a minor matter to extend those results to an arbitrary unidirectional wave packet.) The full Volkov solution in the relativistic Göppert-Mayer gauge is also given in Ref. 15. However, it is not possible to carry out the program leading to an equivalent of the SFA in the Göppert-Mayer gauge. First there is the matter of the cross coupling between the field terms and the atomic potential that appears in Eq. (2.10). The quantity $eA^0$ is very important in the Göppert-Mayer gauge, and so its partial omission in order to reduce the interaction term to $\mathcal{V}^F$ alone constitutes the loss of a major field-dependent term. Furthermore, the Göppert-Mayer Volkov solution is not an eigenstate of $\mathcal{V}^F$, and so the steps analogous to Eqs. (3.7) and (3.8) are not possible.

## IV. NONRELATIVISTIC AND EDA LIMITS

### A. Strong-field approximation

The SFA transition amplitude in Eq. (3.8) will now be taken to the nonrelativistic limit. The four-vector products in Eq. (3.8) are easily converted to three-vector prod-

ucts in the radiation gauge, where $A\cdot p=-\mathbf{A}\cdot\mathbf{p}$ and $A\cdot A=-\mathbf{A}\cdot\mathbf{A}=-\mathbf{A}^2$. The relativistic $\Psi$ and $\Phi$ functions are both normalized in the Klein-Gordon metric, so that the normalization factor is $(2EV)^{-1/2}$, whereas the nonrelativistic Schrödinger counterparts are normalized by $V^{-1/2}$. In the nonrelativistic limit, this introduces an overall $(2m)^{-1}$ into Eq. (3.8), so that the nonrelativistic transition amplitude is

$$(\underline{S}-\underline{1})_{fi}^{\mathrm{SFA}} = -i\int dt\left[\Psi_f^{(-)\mathrm{NR}},\left[-\frac{e\,\mathbf{A}\cdot\mathbf{p}}{m}+\frac{e^2\mathbf{A}^2}{2m}\right]\Phi_i^{\mathrm{NR}}\right]. \tag{4.1}$$

The application of the EDA is permissible in the matrix element, because of the effective limits on radial magnitudes imposed by the bound-state $\Phi$ function. When the EDA is applied, then $\Psi_f^{(-)\mathrm{NR}}$ is identical to what has been used in the past as a so-called "nonrelativistic Volkov solution." The state $\Phi_f^{\mathrm{NR}}$ is the usual nonrelativistic initial-state atomic wave function. Equation (4.1) is then identical to the expression which has been adopted in earlier work[2] as the SFA in the radiation gauge. In this sense, the use of a nominally nonexistent "nonrelativistic Volkov solution" has meaning.

The adoption of Eq. (4.1) as a meaningful transition amplitude is verified by the explicitly relativistic Dirac results.[4,5] These give numerical output in the low- and moderate-intensity domains which is nearly identical to that which emerges from Eq. (4.1). The specific Dirac case which has been evaluated (circular polarization, hydrogenic $1S$ initial state) also gives an analytical nonrelativistic limit identical to that which follows from Eq. (4.1) for that same special case.

### B. Keldysh approximation

As pointed out in Sec. III, there is no transition amplitude in the relativistic Göppert-Mayer gauge equivalent to Eq. (3.8). The Keldysh approximation then remains entirely a physically motivated ansatz nonrelativistic in nature, without a well-defined underlying relativistic formalism. Table I gives a summary of the comparative qualitative properties of the SFA and the Keldysh approximation. It is because of these differences that the phrases "Keldysh type" and "Keldysh style" have been adopted. There *are* clear distinctions between the Keldysh approximation and the SFA.

## V. THE $\mathbf{A}^2$ TERM

### A. Boundary condition considerations

A strategy which has become widespread in multiphoton formalisms is to manipulate the $\mathbf{A}^2$ term, either by complete removal via a contact transformation, or by relocation within the formalism to suit the convenience of the investigator. The basis for these manipulations is that the $\mathbf{A}^2$ term in the EDA is a function only of the time variable. When exponentiated, as it is in the "EDA Volkov solution," it appears to be quite straightforward to remove the $\mathbf{A}^2$ term by a contact transformation.[6–8]

TABLE I. Comparisons between the SFA (strong-field approximation) and the Keldysh approximation.

| SFA | Keldysh approximation |
|---|---|
| Nonrelativistic version published in 1980. Present work gives full, relativistic basis. | Pioneering work. First published in 1964. |
| Rigorous formal basis. | Physically motivated ansatz. |
| SFA is the first term in an expansion in powers of $\mathcal{V}^A$. | Attempt at expansion gives powers of $\mathcal{V}^A-2eA^0V$. |
| All field terms retained at every order. | Some important field terms omitted. |
| In application, use monochromatic approximation (not necessary). | In application, use monochromatic approximation. |
| No further approximations beyond those listed above. | Assume large orders ($n_0\gg1$) in addition to approximations listed above. |
| Two basic intensity parameters: $z=$(ponderomotive potential)/$h\omega$, $z_1=2$ (ponderomotive potential)/(binding energy). | Only one intensity parameter: $\gamma=1/(z_1)^{1/2}$. |
| Supports both low-intensity and high-intensity limits. | Supports high-intensity limit only. |
| Applicable to any initial atomic bound state. | Worked out only for $1S$ hydrogenic initial state. |

This is, in fact, not permissible. As will be shown below, boundary conditions in the photoionization problem require that one of the states in the transition matrix element be free of the external field interaction. Removal of the $\mathbf{A}^2$ term from the interacting state in a Keldysh-type theory then upsets the correct energy conservation condition.

Equation (3.4) is an exact result. It is of a form which is commonplace in several fields of physics. It underlies both the perturbation theory in Sec. III B and the SFA of Sec. III C. Equation (3.4) contains one state with interaction and one without. The $\mathbf{A}^2$-removal strategy corresponds (in the nonrelativistic EDA) to shifting the energy of the state $\Psi_f^{(-)}$ by the amount $e^2\mathbf{A}^2/2mc^2$. However, one must then also shift the energy of the state $\Phi_i$ by the same amount, in which case the $\mathbf{A}^2$ removal is canceled, and nothing is accomplished. If $\mathbf{A}^2$ is removed only from $\Psi_f^{(-)}$, then there is an unbalanced and unphysical energy shift which can have quite spectacular consequences for calculations, as exemplified in Figs. 1–3.

A counterargument made in the atomic physics literature (often implicitly) is that both the initial and final states exhibit the same strong-field dependence, and so removal of the $\mathbf{A}^2$ term should *not* be consequential. The contrast between this point of view and that in the paragraph above then places the entire emphasis on the fundamental formulation of the transition amplitude. The $S$-matrix formalism of Eqs. (3.1)–(3.4) is quite unambiguous in stating that one of the states used in expressing the transition amplitude must be a "reference state," explicitly free of the interaction that causes the transition. Stated in more physical terms, the measurement process appraising the effect of the transition-causing interaction is carried out in an environment free of the interaction Hamiltonian. It is thus appropriate to overlap the fully interacting state onto a noninteracting state in order to evaluate the effect of the interaction. This is done in Eqs. (3.1)–(3.4). Explicitly, it is an appropriate formulation for multiphoton ionization. A transition amplitude formed by the overlap of one completely interacting final state onto another completely interacting initial state corresponds to the making of measurements in a region in which the transition-causing field is still turned on. That is a different process—corresponding to different boundary conditions—than that which is normally measured in

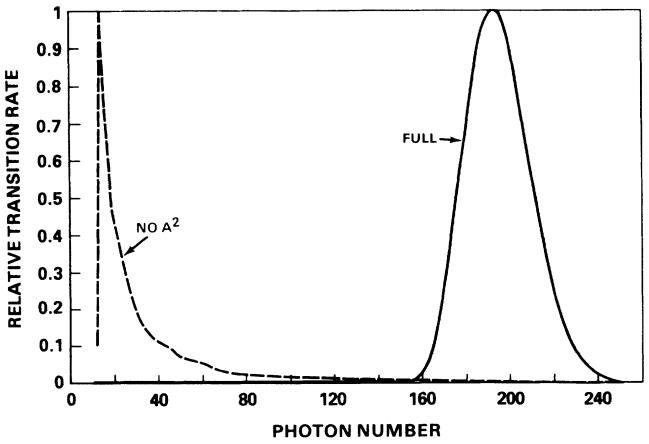


FIG. 2. The photoelectron spectrum is shown for the particular case of $10^{15}$ W/cm$^2$ for the calculational conditions of Fig. 1. Photon number refers to the total number of photons absorbed. The full SFA calculation yields the curve with a smooth peak at large photon number, and the curve with a sharp peak at low photon number shows the results with $\mathbf{A}^2$ removed.

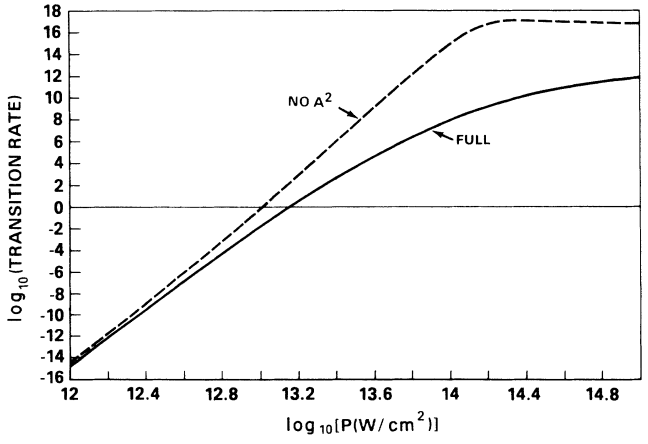


FIG. 1. Calculations of photoionization from the ground state of hydrogen by a circularly polarized laser of 1064 nm wavelength. The log of the total transition rate is plotted against the log of the laser intensity in the range of $10^{12}$–$10^{15}$ W/cm$^2$. The lower curve is from a full SFA calculation with $\mathbf{A}^2$ terms retained, and the upper curve comes about when $\mathbf{A}^2$ is removed.

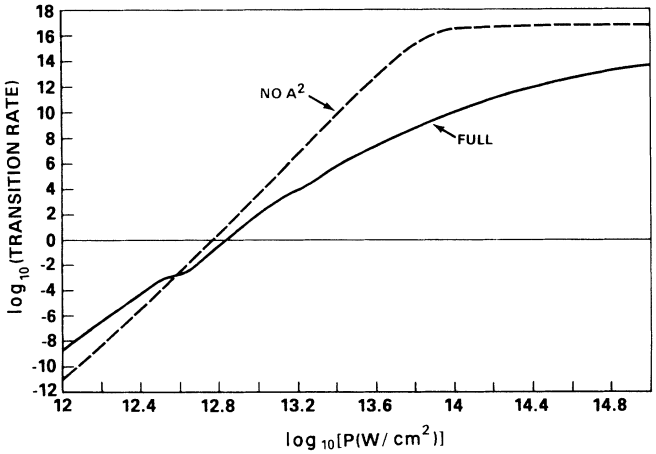


FIG. 3. Calculations of photoionization from the ground state of hydrogen by a linearly polarized laser of 1064 nm wavelength. The log of the total transition rate is plotted against the log of the laser intensity in the range of $10^{12}$–$10^{15}$ W/cm$^2$. The curve which occupies the lower position for most of the graph is from a full SFA calculation with $\mathbf{A}^2$ terms retained, and the curve largely in the upper position comes about when $\mathbf{A}^2$ is removed.

atomic photoionization.

Not all physical problems share the boundary conditions of photoionization. A case in which $\mathbf{A}^2$ terms exactly cancel out between initial and final states is in the Kroll-Watson problem.[16] As was pointed out by Rahman,[17] the Kroll-Watson solution corresponds to a problem in which an atomic potential treated in first order provides a scattering mechanism from one Volkov state to another. That is, the relevant $\underline{S}$ matrix is given by Eq. (3.5) in which $\mathcal{V}^F$ should be replaced by $\mathcal{V}^A$, and the reference states $\Phi$ are both Volkov states. In that case (in the nonrelativistic EDA limit) the $\mathbf{A}^2$ terms from the Volkov states exactly cancel each other, as remarked upon by Rahman.

### B. Relativistic considerations

It was pointed out in the Introduction that sufficiently strong fields require a relativistic theory of photoionization. The notion of $\mathbf{A}^2$ removal cannot then arise, since $A^\mu(x)=A^\mu(\omega t-\mathbf{k}\cdot\mathbf{r})$, and a contact transformation is inapplicable. A calculation carried to completion in a relativistic context is then free of any ambiguity with respect to the treatment of $\mathbf{A}^2$. Such relativistic calculations depend very strongly on the presence of $\mathbf{A}^2$. Explicitly, the circular polarization results shown in Figs. 1 and 2 were done relativistically for those curves that are labeled "full"—meaning with full retention of $\mathbf{A}^2$. The magnitude of the contribution of the $\mathbf{A}^2$ term is evident from Figs. 1 and 2.

At some level of intensity, it should be permissible to ignore relativistic effects. Yet the $\mathbf{A}^2$ term can retain great importance even when the nonrelativistic limit is appropriate. Again in reference to Fig. 2, which is for $10^{15}$ W/cm$^2$ of Nd-YAG (where YAG denotes yttrium aluminum garnet) laser radiation, the nonrelativistic limit is acceptable, since a calculation starting from Eq. (4.1) gives an outcome almost indistinguishable from the complete Dirac calculation.[4,5] When uncertainty exists about how to treat a problem when a limit of any kind is taken, the final arbiter in such decisions is the theory in which that limit is not employed and the full prelimiting theory is consulted. By that rule, the $\mathbf{A}^2$ term must be retained.

### C. Field-interaction considerations

It is argued here that the $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms are two aspects of the same interaction, they are intimately coupled and interchangeable, and hence the neglect of one part of this interaction and retention of the other is fundamentally inconsistent. It is bound to lead to problems in multiphoton processes (except for low-intensity *first-order* processes, where one needs only the $\mathbf{A}\cdot\mathbf{p}$ contribution).

We point out first the fundamental role of $\mathbf{A}^2$ in gauge invariance. The "minimal electromagnetic coupling" substitution $p^\mu\rightarrow p^\mu-eA^\mu$ is introduced on the grounds of gauge invariance. In any theory quadratic in the momentum, as in Schrödinger or Klein-Gordon theory, the $A\cdot A$ or $\mathbf{A}^2$ term is thus a vital part of the proper formulation of the theory. The Dirac theory, even though it is linear in $p^\mu$, provides extra support for this assertion. Because the Dirac formalism never exhibits the $A^2$ term directly, none of the arguments put forward[6–8] for removal of the $A^2$ term can be applied in the Dirac case. Yet the $A^2$ term is implicit in the Dirac theory, hidden by the noncommutative Dirac algebra. Numerical results from Dirac calculations[4,5] fully contain $A^2$ effects. They are consistent with Schrödinger computations from Eq. (4.1) *only* when $\mathbf{A}^2$ terms are retained. Neglect of $\mathbf{A}^2$ violates the manifest gauge invariance inherent in the minimal electromagnetic coupling.

The separate identity of $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms is, in a certain sense, only an illusion. Even after one has selected a particular gauge in which to express the electromagnetic field, conversions between $\mathbf{A}^2$ and $\mathbf{A}\cdot\mathbf{p}$ remain possible. Consider the nonrelativistic, EDA case. In any matrix element containing $\mathbf{A}^2$, if the substitution

$$\mathbf{A}^2=-i[\,\mathbf{A}\cdot\mathbf{r},\,\mathbf{A}\cdot\mathbf{p}] \tag{5.1}$$

is made, along with the usual $\mathbf{p}/m=-i[\mathbf{r},H_0]$, there is an immediate mechanism for exchanging $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ contributions. There is no true distinction between them.

The intimate coupling between $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms becomes very apparent in application of the SFA. To simplify the demonstration as much as possible, consider the nonrelativistic version of the SFA. It is then appropriate to use in the transition matrix element the nonrelativistic version of the Volkov solution given in Eq. (2.6), which is

$$\Psi^{(-)}=V^{-1/2}\exp\left[-iEt+i\mathbf{p}\cdot\mathbf{r}+i\int_t^\infty dt'\left[-\frac{e\,\mathbf{A}\cdot\mathbf{p}}{m}+\frac{e^2\mathbf{A}^2}{2m}\right]\right], \tag{5.2}$$

in which the contributions of the $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms are clearly evident. In the case of a monochromatic field with linear polarization, with $\mathbf{A}=a\boldsymbol{\epsilon}\cos(\omega t)$, the field-dependent exponential in Eq. (5.2) becomes

$$\exp\left[i\int_t^\infty dt'\left[-\frac{e\,\mathbf{A}\cdot\mathbf{p}}{m}+\frac{e^2\mathbf{A}^2}{2m}\right]\right]=\exp\left[i\zeta\sin(\omega t)-i\frac{z}{2}\sin(2\omega t)-iz\omega t\right] \tag{5.3}$$

with the usual asymptotic cutoff, where $\boldsymbol{\epsilon}$ is a unit polarization vector, and where

$$\zeta\equiv ea\,\mathbf{p}\cdot\boldsymbol{\epsilon}/m\omega,\quad z\equiv e^2a^2/4m\omega\ . \tag{5.4}$$

The $z\omega t$ term in the exponential in Eq. (5.3) gives the famous ponderomotive potential or "jitter energy" term in the energy conservation condition.[2,12] Of most immediate interest here are the Floquet terms $\zeta\sin(\omega t)$ and $-(z/2)\sin(2\omega t)$. The first of these arises from the $\mathbf{A}\cdot\mathbf{p}$ term and the second from the $\mathbf{A}^2$ term. They enter directly into energy conservation conditions when it is recognized that these terms constitute a generating function for the generalized Bessel function[18] $J_n(u,v)$,

$$\exp\left[i\left[\zeta\sin(\omega t)-\frac{z}{2}\sin(2\omega t)\right]\right]=\sum_{n=-\infty}^{\infty}e^{in\omega t}J_n\left[\zeta,-\frac{z}{2}\right]. \quad (5.5)$$

The point of Eq. (5.5) is that the $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ contributions are inseparably coupled in the generalized Bessel function. Even as the field intensity becomes small (expressed as $z\to 0$, $\zeta\sim z^{1/2}\to 0$), it is impossible to separate the contributions of $\zeta$ and $z$ terms (i.e., $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms ) except when $n=0,\pm 1$. This is shown in Appendix C of Ref. 2. Hence, $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ are intimately coupled, and cannot be separately treated in multiphoton problems.

The qualifiers in the above conclusions are that the process be of higher-than-first order, and that linear polarization is treated. The same conclusions hold true for all elliptical polarizations except for the special case of circular polarization. For circular polarization, the $\mathbf{A}\cdot\mathbf{p}$ and $\mathbf{A}^2$ terms are not coupled through the generalized Bessel function. All the other remarks about the impropriety of $\mathbf{A}^2$ removal still hold, and it is only as $z\to 0$ that there is a confluence of no-$\mathbf{A}^2$ and with-$\mathbf{A}^2$ circular polarization results, as shown in Figs. 1 and 2. It is important to observe that the linear polarization case continues to show a divergence between no-$\mathbf{A}^2$ and with-$\mathbf{A}^2$ calculations in Fig. 3, even as the intensity becomes small. This is a direct manifestation of the generalized Bessel function coupling shown in Eq. (5.5).

## VI. REMARKS

It has been noted that perturbation theory amounts to the presumption that the atomic potential is stronger than the effects of the applied field, and that the SFA theory is based on the opposite premise. There is an important practical limitation in the application of the SFA approximation. In an energy spectrum of photoelectrons, those spectral peaks at the low-energy end will not have very much kinetic energy, and so they are, in fact, strongly influenced by the atomic potential. One then does not expect the lowest-lying part of the spectrum to be well represented by the SFA approximation. The rule of thumb would be that the SFA should be applicable only for those peaks with kinetic energies of at least a significant fraction of the binding energy. For the ordinary ATI experiments of the past few years, with linearly polarized lasers, this means that the SFA method should not be relied upon for the very important lowest part of the spectrum. That is a serious limitation. There are, however, important areas of strong-field atomic physics where this restriction on the SFA approximation is of little consequence. When circular polarization is used, for all but the lowest ATI intensities the low-energy end of the ATI spectrum is dynamically inhibited,[2,19,20] and so the SFA method works well for the entire observed spectrum. In recent calculations on photoionization from higher-lying states, including Rydberg states, and on photoionization even from ground states with extremely strong fields, those peaks of the spectrum for which the SFA method should be unreliable are only a trivial part of the whole spectrum, even for linear polarization.

## ACKNOWLEDGMENTS

The author is grateful to the Naval Surface Warfare Center, which provided partial support for this research under Contract No. N60921-86-IPA-0477.

## APPENDIX A: THE KLEIN-GORDON $\underline{S}$ MATRIX

The Klein-Gordon $\underline{S}$ matrix found here agrees with that stated by Bjorken and Drell,[13] but it is developed here *ab initio* in a fully covariant way.

The starting point is the basic $\underline{S}$-matrix definition as in Eq. (3.2),

$$S_{fi}=\lim_{t\to+\infty}(\Phi_f,\Psi_i^{(+)}), \quad (A1)$$

$$\lim_{t\to-\infty}\Psi_i^{(+)}=\Phi_i. \quad (A2)$$

These two equations can be combined into

$$(\underline{S}-\underline{1})_{fi}=\lim_{t\to+\infty}(\Phi_f,\Psi_i^{(+)})-\lim_{t\to-\infty}(\Phi_f,\Psi_i^{(+)}). \quad (A3)$$

This is to be used in conjunction with the specification[13] of an inner product in the Klein-Gordon space,

$$(\Phi,\Psi)=\int d^3x\,\Phi^*(i\overleftrightarrow{\partial}^0-2eA^0)\Psi, \quad (A4)$$

along with the definition[13]

$$\Phi^* i\overleftrightarrow{\partial}^0\Psi\equiv\Phi^*(i\partial^0\Psi)-(i\partial^0\Phi^*)\Psi. \quad (A5)$$

Equation (A4) identifies the two terms in Eq. (A3) as surface integrals in the relativistic four-space. Both surfaces are flat, with timelike normal extending along the positive $x^0$ direction in the first term, and the negative $x^0$ direction in the second term. If these surfaces are first taken to be at finite times, with the passage to infinite times taken later, then a closed hypercylindrical solid in four-space can be completed by adding to the two constant-time surfaces a connecting hypercylindrical surface with spacelike normals everywhere. This hypercylinder joins the $t\to+\infty$ surface where it intersects the forward light cone from the origin $x^\mu=0$, and it joins the $t\to-\infty$ surface where it intersects the backward light cone from the origin. The two constant-time surfaces can now be generalized to be of arbitrary configuration confined only by the fact that normals to the surfaces must everywhere be timelike. With these extensions, Eqs. (A3) and (A4) give

$$(\underline{S}-\underline{1})_{fi}=\oint d\sigma_\mu\Phi_f^*(i\overleftrightarrow{\partial}^\mu-2eA^\mu)\Psi_i^{(+)}, \quad (A6)$$

where the double-arrow operator is defined by an immediate extension of Eq. (A5), and where $d\sigma_\mu$ is a four-surface element of area on the above-described closed hypersolid with outwardly directed normal. Inherent in the passage from Eq. (A3) to (A6) is the notion that the state vectors vanish at large spacelike displacements from the origin. This limit (and the entire procedure just outlined) is the same as that used in the standard demonstration of

the continuity condition in relativistic quantum mechanics. Equation (A6) can be written as

$$(\underline{S}-\underline{1})_{fi}=\oint d\sigma_\mu J^\mu \ , \tag{A7}$$

where $J^\mu$ is a "transition current" defined by the correspondence of Eq. (A7) to (A6). By the four-divergence theorem, this can be restated as

$$(\underline{S}-\underline{1})_{fi}=-i\int d^4x(i\partial_\mu J^\mu) \ . \tag{A8}$$

The result of acting on $J^\mu$ with $i\partial_\mu$ can be rearranged by employing the difference of the two expressions

$$\Phi_f^*[(i\partial_\mu-eA_\mu)(i\partial^\mu-eA^\mu)-m^2]\Psi_i^{(+)}=0 \ , \tag{A9}$$

$$[(i\partial_\mu i\partial^\mu-m^2)\Phi_f^*]\Psi_i^{(+)}=0 \ , \tag{A10}$$

which follow from the equations of motion. After a bit of algebra and an integration by parts, the result is

$$(\underline{S}-\underline{1})_{fi}=-i\int d^4x\ \Phi_f^* \times(i\partial_\mu eA^\mu+eA^\mu i\partial_\mu-e^2A\cdot A)\Psi_i^{(+)} \ , \tag{A11}$$

or, with the terminology of Eq. (2.4),

$$(\underline{S}-\underline{1})_{fi}=-i\int d^4x\ \Phi_f^*\mathcal{V}_{\rm KG}\Psi_i^{(+)} \ . \tag{A12}$$

The time-reversed $\underline{S}$ matrix, by exactly the same procedures, is

$$(\underline{S}-\underline{1})_{fi}=-i\int d^4x\ \Psi_f^{(-)*}\mathcal{V}_{\rm KG}\Phi_i \ . \tag{A13}$$

## APPENDIX B: THE $\underline{S}$ MATRIX AND FERMI'S GOLDEN RULE

Fermi's golden rule[21] will now be derived from the $\underline{S}$-matrix formalism. This can be done without reference to perturbation theory. Consider first a nonrelativistic time-independent problem in which transitions are caused by an interaction Hamiltonian $V$. Then, with $\hbar$ restored for this work, the starting point is the $\underline{S}$-matrix expression

$$(\underline{S}-\underline{1})=-(i/\hbar)\int dt(\Phi_f,V\Psi_i^{(+)}) \ . \tag{B1}$$

Since the problem is stationary, the states can be written as

$$\Phi_f=\phi_f\exp(-iE_ft/\hbar),\quad \Psi_i^{(+)}=\psi_i^{(+)}\exp(-iE_it/\hbar) \ . \tag{B2}$$

When Eq. (B2) is substituted into (B1), the time integration can be done, yielding

$$(\underline{S}-\underline{1})_{fi}=-2\pi i\delta(E_f-E_i)T_{fi} \ , \tag{B3}$$

where the $\underline{T}$ matrix,

$$T_{fi}=(\phi_f,V\psi_i) \tag{B4}$$

is generally viewed as being defined by Eq. (B3).

From the way in which the $\underline{S}$ matrix is introduced as a transition amplitude, the transition probability per unit time for a transition is

$$w=\lim_{\tau\to\infty}\frac{|S_{fi}-\delta_{fi}|^2}{\tau}=\lim_{\tau\to\infty}\frac{2\pi\delta(E_f-E_i)2\pi\delta(0)}{\tau}|T_{fi}|^2 \ , \tag{B5}$$

using Eq. (B3) and the general result on the product of the $\delta$ functions that $\delta(x-a)f(x)=\delta(x-a)f(a)$. With the $\delta$-function representation

$$2\pi\delta(E_f-E_i)=\lim_{\tau\to\infty}\int_{-\tau/2}^{\tau/2}dt\frac{1}{\hbar}\exp[i(E_f-E_i)t/\hbar] \ , \tag{B6}$$

then

$$2\pi\delta(0)=\lim_{\tau\to\infty}\int_{-\tau/2}^{\tau/2}dt\frac{1}{\hbar}=\frac{\tau}{\hbar} \ , \tag{B7}$$

and so

$$w=(2\pi/\hbar)\delta(E_f-E_i)|T_{fi}|^2 \ . \tag{B8}$$

For transitions into a continuum of final states, the total transition rate is

$$W=\frac{2\pi}{\hbar}\int_{E_f-\Delta E/2}^{E_f+\Delta E/2}dE\ \delta(E_f-E_i)|T_{fi}|^2\rho(E) \ , \tag{B9}$$

where $\rho(E)$ is the density of final states. This then gives Fermi's golden rule

$$W=(2\pi/\hbar)|T_{fi}|^2\rho(E) \tag{B10}$$

in terms of the $\underline{T}$ matrix of Eq. (B4).

The above results will now be extended to time-dependent problems. At the same time, since little extra complication is involved, the states are presumed to possess uniformly spaced sidebands in the presence of the applied field. This is Floquet behavior, and it is the nature of the SFA method when the field is taken to be monochromatic. Then the $\underline{S}$ matrix is of the form

$$(\underline{S}-\underline{1})_{fi}=-2\pi i\sum_n\delta(\Delta E-n\hbar\omega)T_{fi}^{(n)} \ , \tag{B11}$$

which generalizes Eq. (B3). Specifically, in ATI problems,

$$\Delta E=E_f-E_i+z\hbar\omega \ , \tag{B12}$$

in the notation of Ref. 2, where $z$ is the basic dimensionless intensity parameter and $z\hbar\omega$ is the ponderomotive potential. Equation (B5) now becomes

$$w=\lim_{\tau\to\infty}\frac{|S_{fi}-1|^2}{\tau}=\sum_n\frac{2\pi\delta(\Delta E-n\hbar\omega)2\pi\delta(0)}{\tau}|T_{fi}^{(n)}|^2 \ , \tag{B13}$$

in which all cross terms of $\delta$ functions with different arguments explicitly vanish. The analog of Eq. (B8) is then

$$w=(2\pi/\hbar)\sum_n\delta(\Delta E-n\hbar\omega)|T_{fi}^{(n)}|^2 \ . \tag{B14}$$

The step analogous to Eq. (B9) is carried out in Ref. 2 by integration over the phase space of the detached electrons in order to arrive at $W$, the total transition rate.

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