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# Gauge-independent Wigner functions: General formulation

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We introduce a gauge-invariant Wigner operator (GIWO) and a gauge-independent Wigner function (GIWF) that allow for both quantized and classical electromagnetic fields. If only classical fields are present, a Weyl transform analogous to the one associated with ordinary Wigner functions can be defined for any operator; in the case of quantized fields this is at least possible for Weyl-ordered functions of the position and kinetic momentum operators. We show how the evolution of the operators having a Weyl transform can be followed with the aid of the GIWF defined as the Heisenberg-picture expectation value of the GIWO, and derive for the GIWO the Heisenberg equation of motion which only involves the physical electric and magnetic fields. Some aspects of the case of entirely classical fields are discussed in more detail. (i) The GIWF in conjunction with the postulate that physical observables can be measured without referring to the gauge permits a quantum-mechanical treatment of a full experimental run without the problem of relating the measured values to the gauge-dependent density operator. (ii) A closed equation of motion for the GIWF is obtained. (iii) In the dipole approximation quantum features of the dynamics are lost. (iv) Quantum corrections to dynamics are associated with recoil effects.

## I. INTRODUCTION

The Wigner function[1] (WF) and related quasiprobability distributions allow quantum-mechanical expectation values to be written as phase-space integrals analogous to those of classical mechanics. Classical intuition may then be taken over to quantum mechanics, and semiclassical $\hbar$ or $1/T$ expansions can be carried out remarkably easily.[1-5] Applications of the WF along these lines have emerged in wildly varying fields of physics and theoretical chemistry; we mention as an example the formulation of collision theory in terms of the WF.[6] Lorentz-covariant forms of the WF may also be envisaged. Accordingly, applications to relativistic quantum statistical mechanics have been proposed.[2,7] Finally, quasiprobability distributions permit mappings of operator equations onto $c$-number relations, which is the source of their use in quantum optics.[8]

Studies of photon recoil effects[9-12] on an atom constitute one particular application of the WF to $\hbar$ expansions. The initial motivation of this work was to develop a similar WF treatment of the motion of an unbound charged particle in an electromagnetic (EM) field. Although an immense literature has accumulated around the motion of an electron in electric and magnetic fields, WF methods similar to those we have in mind are scarce.[13-15] In fact, the ordinary WF stumbles on two fundamental obstacles: In atoms the dipole approximation can be used, and hence problems of gauge invariance are averted.[16-18] A dipole approximation can also be introduced for an unbound electron by neglecting the spatial variation of the radiation field, but then the photon momentum is simultaneously forced to be zero. Consequently, the Doppler shift and recoil effects are lost. Avoiding the dipole approximation seems desirable, but then special care must be taken in order not to generate gauge-dependent results. The ordinary WF is gauge dependent and does not suit to this aim. Second, while in atoms spontaneous emission is easy to deal with, it seems to us that it has not been known how to incorporate the quantized radiation reaction field[19] into the WF of a charged particle.

In this paper we present a gauge-invariant Wigner operator (GIWO) and a gauge-independent Wigner function (GIWF) for a charged particle in an EM field that also includes the quantized modes of radiation, and derive the Heisenberg equation of motion for the GIWO. In a follow-up paper[20] this and the equation of motion for the EM field are combined to gain access to radiation reaction fields, which will lead to relaxation terms in the equation of motion of the GIWF.

In order to set the stage for the development to follow we summarize some aspects of the ordinary WF for one nonrelativistic particle.[2-5] We define a collection of functions of the canonical position and momentum operators $\hat{r}$ and $\hat{p}$, labeled by classical indices $r$ and $p$, as

$$\hat{W}(r,p)=\frac{1}{(2\pi\hbar)^6}\int d^3u\, d^3v \exp\left[\frac{i}{\hbar}[u\cdot(\hat{p}-p)+v\cdot(\hat{r}-r)]\right]. \quad (1.1)$$

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(See Ref. 21 for a comment on the notation used here.) Since every operator function[22] of $\hat{r}$ and $\hat{p}$ can obviously be represented as a linear combination of the "Wigner operators" (WO's) $\hat{W}(r,p)$ in the form

$$\hat{O}(\hat{r},\hat{p})=\int d^3r\,d^3p\,O(r,p)\hat{W}(r,p)\ , \tag{1.2}$$

$\{\hat{W}(r,p)\}_{r,p}$ can be viewed as a basis in the space of one-particle operators, and the classical function $O(r,p)$ serves as a continuous set of expansion coefficients. Because

$$\mathrm{Tr}[\hat{W}(r,p)\hat{W}(r',p')]=(2\pi\hbar)^{-3}\delta(p-p')\delta(r-r')\ , \tag{1.3}$$

a one-to-one correspondence between the operators $\hat{O}$ and the expansion coefficients $O$ can be set up:

$$\hat{O}(\hat{r},\hat{p})\leftrightarrow O(r,p)=(2\pi\hbar)^3\mathrm{Tr}[\hat{W}(r,p)\hat{O}(\hat{r},\hat{p})]\ . \tag{1.4}$$

The function $O$ is called[23,24] the Weyl transform of the operator $\hat{O}$. If the operator $\hat{O}(\hat{r},\hat{p})$ is given by a power series of Weyl-ordered (i.e., totally symmetrized) products of the operators $\hat{r}_i,\hat{p}_i$,

$$\hat{O}(\hat{r},\hat{p})=\sum_{\substack{m_1,m_2,m_3\\ n_1,n_2,n_3}} A^{m_1m_2m_3}_{n_1n_2n_3}\{\hat{r}_1^{m_1}\hat{r}_2^{m_2}\hat{r}_3^{m_3}\hat{p}_1^{n_1}\hat{p}_2^{n_2}\hat{p}_3^{n_3}\}_W\ , \tag{1.5}$$

then its Weyl transform $O(r,p)$ is precisely the same function of the $c$-number variables $r_i$ and $p_i$,

$$O(r,p)=\sum A^{m_1m_2m_3}_{n_1n_2n_3} r_1^{m_1}r_2^{m_2}r_3^{m_3}p_1^{n_1}p_2^{n_2}p_3^{n_3}\ . \tag{1.6}$$

Although such a simple substitution is not valid for a general operator ordering, we stress that the Weyl transform still exists and is given by (1.4). For instance, using the commutators of $\hat{r}$ and $\hat{p}$ and (1.5) and (1.6) we obtain

$$\hat{r}_1\hat{p}_1=\tfrac{1}{2}(\hat{r}_1\hat{p}_1+\hat{p}_1\hat{r}_1)+\frac{i\hbar}{2}\leftrightarrow r_1p_1+\frac{i\hbar}{2}\ . \tag{1.7}$$

Letting $\hat{\rho}$ denote the density operator of the particle, it follows from (1.2) that

$$\mathrm{Tr}(\hat{O}\hat{\rho})=\int d^3r\,d^3p\,O(r,p)\mathrm{Tr}[\hat{W}(r,p)\hat{\rho}]$$
$$=\int d^3r\,d^3p\,W(r,p)O(r,p)\ , \tag{1.8}$$

where the WF $W(r,p)$ is defined as

$$W(r,p)=\mathrm{Tr}[\hat{W}(r,p)\hat{\rho}]$$
$$=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}u\cdot p\right]\langle r-\tfrac{1}{2}u\,|\hat{\rho}|\,r+\tfrac{1}{2}u\,\rangle\ . \tag{1.9}$$

The quantum-mechanical expectation value of the operator $\hat{O}$ may thus be computed just like a classical expectation value as an integral over phase space, provided $\hat{O}$ is replaced with its Weyl transform $O$ and $\hat{\rho}$ with the WF $W$. However, the WF is not a true phase-space density. It is real, but it may take on negative values. In fact, the WF corresponding to a pure state $\hat{\rho}=|\psi\rangle\langle\psi|$ is nonnegative if and only if the wave function $\langle r\,|\,\psi\rangle$ is an exponential of a quadratic polynomial of $r_1$, $r_2$, and $r_3$.[25] As $\hat{\rho}$ is a positive operator, the procedure (1.9) cannot produce arbitrary functions of $r$ and $p$, and hence all classical phase-space distributions are not valid Wigner functions either. An example would be $W(r,p)=\delta(r)\delta(p)$, which is feasible in classical mechanics but would give $\Delta p\Delta x=0$ in quantum mechanics, too.

With the Hamiltonian

$$\hat{H}=\frac{\hat{p}^2}{2M}+\hat{V}(\hat{r}) \tag{1.10}$$

the Liouville—von Neumann equation for the density operator $\hat{\rho}$ leads to the equation of motion for the WF:

$$\left\{\frac{\partial}{\partial t}+\frac{p}{M}\cdot\frac{\partial}{\partial r}-\frac{\partial}{\partial p}\cdot\int_{-1/2}^{1/2}d\tau\left[\frac{\partial}{\partial r}V\left[r+i\hbar\tau\frac{\partial}{\partial p}\right]\right]\right\}$$
$$\times W(r,p,t)=0\ . \tag{1.11}$$

Here the operator inside the integral is obtained by first forming the $\partial/\partial r$ derivative of $V$, and then inserting the appropriate arguments. This equation allows one to follow the evolution of the expectation values of all operators. If $V$ is at most a quadratic function of $r_i$, (1.11) becomes the classical Liouville equation. In this case the difference between classical mechanics and quantum mechanics no longer shows in the dynamics of the distribution function, but it is still buried in three places in the formalism.[3] First, the function spaces where the distribution functions are allowed to reside are different. Second, the Wigner function may depend explicitly on $\hbar$. Third, the Weyl transform of an operator may depend explicitly on $\hbar$.

In the presence of a magnetic field when the vector potential $\hat{A}(\hat{r})$ cannot be chosen to vanish, a variant of the WF giving the expectation values of functions of the gauge-invariant kinetic momentum $\hat{k}=\hat{p}-Q\hat{A}(\hat{r})$ according to the prescription (1.5), (1.6), and (1.8) would be more appropriate than the WF for the operator $\hat{p}$. Even if the EM field is not quantized, such a function is *not* obtained by simply transforming the variable $p$ to $k=p-QA(r)$ in the WF; see the Appendix. Instead, one can define

$$W(r,k)=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}u\cdot\left[k+Q\int_{-1/2}^{1/2}d\tau\,A(r+\tau u)\right]\right]\langle r-\tfrac{1}{2}u\,|\hat{\rho}|\,r+\tfrac{1}{2}u\,\rangle \tag{1.12}$$

as a suitable GIWF.[26–28] Although this form has been known for a long time, to our knowledge considerations like those sketched above for the ordinary WF have not been published for the GIWF—not even the full equation of motion in a form that would display the similarities to and differences from the classical Liouville equation. Our first aim is to fill this gap. Our second task is to generalize (1.12) further by letting $\hat{A}(\hat{r})$ be an operator of the quantized EM field.

The outline of the present paper is the following. In Sec. II we define the GIWO, and the GIWF as the expectation value of the GIWO. The generalizations of properties (1.1)–(1.9) to the GIWO and GIWF for both classical and quantized EM fields, with a special emphasis on the differences between these two cases, are presented in Sec. III. In Sec. IV we derive the Heisenberg equation of motion for the GIWO, and show how this determines the evolution of the expectation values of observables. The brief analysis of the case with only classical fields in Sec. V serves as a first demonstration of the results of our formulation. The discussion in Sec. VI concludes the paper. In the Appendix we briefly consider an alternative suggestion to include the vector potential into the WF.

## II. THE WIGNER OPERATOR AND THE WIGNER FUNCTION

### A. Basic notation

We study a nonrelativistic particle with mass $M$ and charge $Q$ in the whole three-dimensional space $\mathbb{R}^3$ (which excludes the Aharonov-Bohm effect[29]). The canonical position and momentum operators $\hat{r}$ and $\hat{p}$ furnish a complete set of operators for the spatial motion of the particle. From the commutator

$$[\hat{r}_i,\hat{p}_j]=i\hbar\delta_{ij} \tag{2.1}$$

it follows that the corresponding eigenvectors $|r\rangle,|p\rangle$ may be chosen to satisfy

$$\hat{r}\,|r\rangle=r\,|r\rangle,\ \ \hat{p}\,|p\rangle=p\,|p\rangle\ , \tag{2.2a}$$

$$\langle r\,|r'\rangle=\delta(r-r'),\ \ \langle p\,|p'\rangle=\delta(p-p')\ , \tag{2.2b}$$

$$\int d^3r\,|r\rangle\langle r\,|=1,\ \ \int d^3p\,|p\rangle\langle p\,|=1\ , \tag{2.2c}$$

$$\langle r\,|p\rangle=\frac{1}{(2\pi\hbar)^{3/2}}\exp\left[\frac{i}{\hbar}p\cdot r\right]\ . \tag{2.2d}$$

The particle interacts with an electromagnetic field as yet specified by the scalar potential $\hat{\Phi}(\hat{r},t)$ and the vector potential $\hat{A}(\hat{r},t)$. For maximum flexibility we adopt the semiclassical approach,[30] so the latter may contain both classical field modes and modes of the quantized field,

$$\hat{A}(\hat{r},t)=\hat{A}_C(\hat{r},t)+\hat{A}_Q(\hat{r})\ . \tag{2.3}$$

The classical field might be given in any gauge, but according to the established practice we use the radiation gauge whenever a quantized field is present. In terms of boson operators $\hat{b}_q$ that annihilate photons with momentum $\hbar q$, frequency $\Omega_q$, and linear polarization $\epsilon(q)$ (the polarization label $\sigma=1,2$ is implicitly included in the wave vector $q$ even when not shown), the radiation field is given in the Schrödinger picture by

$$\hat{A}_Q(\hat{r})=\hat{A}^{(+)}(\hat{r})+\hat{A}^{(-)}(\hat{r})\ , \tag{2.4a}$$

$$\hat{A}^{(+)}(\hat{r})=-i\sum_q{}'g(q)\hat{b}_q e^{iq\cdot\hat{r}},\ \ \hat{A}^{(-)}=(\hat{A}^{(+)})^\dagger\ , \tag{2.4b}$$

$$g(q)=\left[\frac{\hbar}{2\Omega_q\epsilon_0V}\right]^{1/2}\epsilon(q)\ . \tag{2.4c}$$

The primed sum runs over the quantized field modes.

We now pause to prove an auxiliary result that is going to play a considerable role in our theory: For any classical vectors $u,v$ and for any Cartesian coordinates $i,j=1,2,3$ the commutator

$$[\hat{A}_i(\hat{r}+u),\hat{A}_j(\hat{r}+v)]=0 \tag{2.5}$$

holds true. To establish this, we temporarily invoke the polarization labels in the expression (2.4) of the field. From the commutators

$$[\hat{b}_{q,\sigma},\hat{b}^\dagger_{q',\sigma'}]=\delta_{q,q'}\delta_{\sigma,\sigma'}\ ,\qquad [\hat{b}_{q,\sigma},\hat{b}_{q',\sigma'}]=[\hat{b}^\dagger_{q,\sigma},\hat{b}^\dagger_{q',\sigma'}]=0 \tag{2.6}$$

it follows that

$$[\hat{A}_i(\hat{r}+u),\hat{A}_j(\hat{r}+v)]=\sum_{q,\sigma}{}'\frac{\hbar}{2\Omega_q\epsilon_0V}\epsilon_i^\sigma(q)\epsilon_j^\sigma(q)\{\exp[iq\cdot(u-v)]-\exp[-iq\cdot(u-v)]\}\ . \tag{2.7}$$

The polarization vectors may be chosen in such a way that $\epsilon_i^{1,2}(q)=\epsilon_i^{2,1}(-q)$. It can then be seen that if there were no restrictions on the sum in (2.7), it would consist of two subsums which cancel. The assumedly finite number of modes which are treated classically are excluded in the sum in (2.7), but then the cancellation only fails up to a contribution of the order $1/V$ that goes to zero with $V\rightarrow\infty$. Besides, it could be demonstrated from a full quantum treatment that the restriction on the sum is an artifact. Hence (2.5) is verified.

The classical electric and magnetic fields are obtained from the classical potentials through

$$\hat{E}_C(\hat{r},t)=-\frac{\partial}{\partial\hat{r}}\Phi(\hat{r},t)-\frac{\partial}{\partial t}\hat{A}_C(\hat{r},t)\ , \tag{2.8}$$

$$\hat{B}_C(\hat{r},t)=\frac{\partial}{\partial\hat{r}}\times\hat{A}_C(\hat{r},t)\ , \tag{2.9a}$$

or writing the latter in component form with the aid of the Levi-Civita symbol $\epsilon_{ijk}$,

$$\hat{B}_{C,k}=\sum_{i,j}\epsilon_{ijk}\frac{\partial}{\partial\hat{r}_i}\hat{A}_{C,j}\ . \tag{2.9b}$$

Here and below a derivative with respect to an operator of a function of this operator is understood as the derivative of the function in question with the operator argument,

$$\frac{\partial}{\partial\hat{r}_i}\hat{A}_j(\hat{r})=\frac{\partial}{\partial r_i}A_j(r)\bigg|_{r=\hat{r}}\ , \tag{2.10a}$$

or equivalently,

$$\frac{\partial}{\partial\hat{r}_i}\hat{A}_j(\hat{r})=\frac{\partial}{\partial u_i}\hat{A}_j(\hat{r}+u)\bigg|_{u=0}\ . \tag{2.10b}$$

By comparing (2.10b) and (2.5) it can be seen that (2.5) also holds for arbitrary spatial derivatives of the vector potential, in particular for the magnetic field and its derivatives.

The counterparts of (2.8) and (2.9) for the quantized fields can be written

$$\hat{E}_Q^{(+)}(\hat{r})=\sum_q{}' \Omega_q g(q)\hat{b}_q \exp(iq\cdot\hat{r}) \,, \tag{2.11}$$

$$\hat{B}_Q^{(+)}(\hat{r})=\sum_q{}' q\times g(q)\hat{b}_q \exp(iq\cdot\hat{r}) \,. \tag{2.12}$$

We have displayed explicitly only the positive-frequency parts of the operators. The negative-frequency parts are simply Hermitian conjugates of these, and the full quantum fields are sums of the positive- and negative-frequency parts. The full fields, finally, are sums of classical and quantized fields, e.g.,

$$\hat{B}(\hat{r},t)=\hat{B}_C(\hat{r},t)+\hat{B}_Q(\hat{r}) \,. \tag{2.13}$$

We next introduce the kinetic momentum operator

$$\hat{k}=\hat{p}-Q\hat{A}(\hat{r},t) \,. \tag{2.14}$$

Its commutators read

$$[\hat{r}_i,\hat{k}_j]=i\hbar\delta_{i,j}, \quad [\hat{k}_i,\hat{k}_j]=i\hbar Q\sum_k \epsilon_{ijk}\hat{B}_k(\hat{r},t) \,. \tag{2.15}$$

In contrast to the canonical momentum $\hat{p}$, different components of the kinetic momentum $\hat{k}$ do not commute, and the commutator may even be a quantum-field operator.

### B. Definition of the Wigner operator

We define "the generating operator"

$$\hat{T}(u,v)\equiv\exp\left[\frac{i}{\hbar}(u\cdot\hat{k}+v\cdot\hat{r})\right] \tag{2.16}$$

and the GIWO $\hat{W}(r,k)$ as the Fourier transform of $\hat{T}(u,v)$,

$$\hat{W}(r,k)=\frac{1}{(2\pi\hbar)^6}\times\int d^3u\, d^3v \exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right]\hat{T}(u,v) \,. \tag{2.17}$$

This is completely analogous to (1.1). Next, letting $\hat{\rho}$ denote the density operator for the quantized degrees of freedom for the system particle + field, we define the GIWF just like in (1.9),

$$W(r,k)=\mathrm{Tr}[\hat{W}(r,k)\hat{\rho}] \,. \tag{2.18}$$

The GIWF is thus the expectation value of the GIWO. Notice that the GIWO is Hermitian and the GIWF is real. To the extent that the GIWF can be interpreted as a distribution function, the expectation value of the operator $\hat{T}$ is the characteristic function of the distribution.

Since the implications of these definitions are somewhat different depending on whether quantized fields are present or not, we discuss these cases separately in Secs. III A and III B. Meanwhile we complete the introduction of the basic mathematical machinery needed to deal with the GIWO.

### C. Baker-Campbell-Hausdorff formulas

We now derive a number of Baker-Campbell-Hausdorff (BCH) formulas that recur over and over in the sequel. First note that by taking the matrix elements of the operators involved one can prove from (2.2) the relations

$$\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]|r\rangle=|r-u\rangle \,, \tag{2.19a}$$

$$\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]f(\hat{r})=f(\hat{r}+u)\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right] , \tag{2.19b}$$

as is natural since $\hat{p}$ is the generator of spatial translations.

Let us next study the operator

$$\hat{T}(u,v;\tau)=\exp\left[\frac{i}{\hbar}\tau(u\cdot\hat{k}+v\cdot\hat{r})\right]=\exp\left[\frac{i}{\hbar}\tau[u\cdot\hat{p}+v\cdot\hat{r}-Qu\cdot\hat{A}(\hat{r})]\right] . \tag{2.20}$$

With $\tau=1$ this becomes the operator $\hat{T}(u,v)$ of (2.16), i.e., the Fourier transform of the GIWO. Taking the derivative of (2.20) with respect to $\tau$ gives

$$\frac{\partial}{\partial\tau}\hat{T}(\tau)=\frac{i}{\hbar}\{u\cdot\hat{p}+[v\cdot\hat{r}-Qu\cdot\hat{A}(\hat{r})]\}\hat{T}(\tau) \,, \tag{2.21a}$$

and clearly

$$\hat{T}(0)=1 \,. \tag{2.21b}$$

Transforming to an "interaction picture" with

$$\hat{T}(\tau)=\exp\left[\frac{i}{\hbar}\tau u\cdot\hat{p}\right]\hat{T}'(\tau) \,, \tag{2.22}$$

we obtain from (2.21) and (2.19b) the equation for $\hat{T}'(\tau)$:

$$\frac{\partial}{\partial\tau}\hat{T}'=\frac{i}{\hbar}[v\cdot(\hat{r}-\tau u)-Qu\cdot\hat{A}(\hat{r}-\tau u)]\hat{T}'(\tau) \,, \tag{2.23a}$$

$$\hat{T}'(0)=1 \,. \tag{2.23b}$$

Since only commuting operators appear inside the square brackets in (2.23a), the solution to (2.23) can be found immediately,

$$\hat{T}'(\tau)=\exp\left\{\frac{i}{\hbar}\left[\tau v\cdot\left[\hat{r}-\frac{\tau}{2}u\right]-Qu\cdot\int_0^\tau d\tau\,\hat{A}(\hat{r}-\tau u)\right]\right\} . \tag{2.24}$$

With $\tau=1$, a formula for $\hat{T}(u,v)$ in (2.16) follows from (2.22) and (2.24). With the aid of (2.19b) the result may be cast into several useful forms:

$$\hat{T}(u,v)=\exp\left[-\frac{i}{2\hbar}u\cdot v\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}-\tau u)\right]\right] \tag{2.25a}$$

$$=\exp\left[\frac{i}{2\hbar}u\cdot\hat{p}\right]\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_{-1/2}^{1/2} d\tau\,\hat{A}(\hat{r}+\tau u)\right]\right]\exp\left[\frac{i}{2\hbar}u\cdot\hat{p}\right] \tag{2.25b}$$

$$=\exp\left[\frac{i}{2\hbar}u\cdot v\right]\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}+\tau u)\right]\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]. \tag{2.25c}$$

Further BCH formulas that are used later can be derived in a similar way:

$$\hat{T}(u,v)=\exp\left[\frac{i}{2\hbar}u\cdot v\right]\exp\left[\frac{i}{\hbar}v\cdot\hat{r}\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right] \tag{2.26a}$$

$$=\exp\left[-\frac{i}{2\hbar}u\cdot v\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]\exp\left[\frac{i}{\hbar}v\cdot\hat{r}\right], \tag{2.26b}$$

$$\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]=\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}+\tau u)\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right] \tag{2.27a}$$

$$=\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}-\tau u)\right]. \tag{2.27b}$$

We finally emphasize that all BCH formulas presented are valid regardless of whether quantized fields are present or not. This follows directly from (2.5).

## III. PROPERTIES OF THE GIWF

### A. The case of classical fields

In this section we discuss the case when only classical EM fields are present. Then $\hat{\Phi}(\hat{r},t)$ and $\hat{A}(\hat{r},t)$ are operators only through their argument $\hat{r}$, and the vectors $|r\rangle$ (or $|p\rangle$) form a complete basis for the quantum-mechanical part of the problem.

We first derive an expression for the GIWF from (2.18) using the BCH formula (2.25b). We obtain

$$\mathrm{Tr}[\hat{T}(u,v)\hat{\rho}]=\int d^3r\left\langle r\left|\exp\left[\frac{1}{2\hbar}u\cdot\hat{p}\right]\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_{-1/2}^{1/2}d\tau\,\hat{A}(\hat{r}+\tau u)\right]\right]\exp\left[\frac{i}{2\hbar}u\cdot\hat{p}\right]\hat{\rho}\right|r\right\rangle \tag{3.1a}$$

$$=\int d^3r\left\langle r\left|\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_{-1/2}^{1/2}d\tau\,\hat{A}(\hat{r}+\tau u)\right]\right]\exp\left[\frac{i}{2\hbar}u\cdot\hat{p}\right]\hat{\rho}\exp\left[\frac{i}{2\hbar}u\cdot\hat{p}\right]\right|r\right\rangle \tag{3.1b}$$

$$=\int d^3r\,\exp\left[\frac{i}{\hbar}\left[v\cdot r-Qu\cdot\int_{-1/2}^{1/2}d\tau\,A(r+\tau u)\right]\right]\langle r+\tfrac{1}{2}u\,|\hat{\rho}|\,r-\tfrac{1}{2}u\rangle, \tag{3.1c}$$

where (3.1b) follows from the cyclic invariance of the trace and (3.1c) from (2.19a) and its Hermitian conjugate. Taking the Fourier transform we obtain the GIWF,

$$W(r,k)=\frac{1}{(2\pi\hbar)^6}\int d^3u\,d^3v\,\exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right]\mathrm{Tr}[\hat{T}(u,v)\hat{\rho}]$$

$$=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}u\cdot\left[k+Q\int_{-1/2}^{1/2}d\tau\,A(r+\tau u)\right]\right]\langle r-\tfrac{1}{2}u\,|\hat{\rho}|\,r+\tfrac{1}{2}u\rangle, \tag{3.2}$$

which coincides with the earlier definitions[26-28] reproduced in (1.12).

Starting from (2.25a) and (2.25c) we obtain in a similar way

$$\mathrm{Tr}[\hat{T}(u,v)\hat{T}(u',v')]=(2\pi\hbar)^3\delta(u+u')\delta(v+v'). \tag{3.3}$$

Carrying out the relevant Fourier transforms we find that the GIWO satisfies the exact counterpart of (1.3) for the ordinary WO,

$$\mathrm{Tr}[\hat{W}(r,k)\hat{W}(r',k')]=(2\pi\hbar)^{-3}\delta(r-r')\delta(k-k'). \tag{3.4}$$

Since $\{\hat{r},\hat{p}\}$ is a complete set of one-particle operators, so is obviously $\{\hat{r},\hat{k}\}$. Let us now assume that a given operator $\hat{O}$ can be represented in the form analogous to (1.2) as

$$\hat{O}(\hat{r},\hat{k})=\int d^3r\, d^3k\, O(r,k)\hat{W}(r,k)\ . \tag{3.5}$$

We do not try to determine the class of operators that are amenable to the representation (3.5) with sufficiently well-behaved "functions" $O(r,k)$ (a clear exposition of possible problems is presented in Ref. 5), but merely assume that the class is large enough for our purposes. By virtue of (3.4), a Weyl correspondence analogous to (1.4) can then be set up,

$$\hat{O}(\hat{r},\hat{k})\leftrightarrow O(r,k)=(2\pi\hbar)^3\mathrm{Tr}[\hat{W}(r,k)\hat{O}(\hat{r},\hat{k})]\ . \tag{3.6}$$

Since (3.5) may formally be written as

$$\hat{O}(\hat{r},\hat{k})=\frac{1}{(2\pi\hbar)^6}\int d^3u\, d^3v\left[\int d^3r\, d^3k \exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right]O(r,k)\exp\left[\frac{i}{\hbar}(u\cdot\hat{k}+v\cdot\hat{r})\right]\right]$$
$$=\frac{1}{(2\pi\hbar)^6}\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{i}{\hbar}\right]^n\int d^3u\, d^3v(u\cdot\hat{k}+v\cdot\hat{r})^n\left[\int d^3r\, d^3k\exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right]O(r,k)\right], \tag{3.7}$$

and the expansion of the powers in (3.7) automatically produces all possible orderings of the operators $\hat{k}_i,\hat{r}_i$, the operator $\hat{O}(\hat{r},\hat{k})$ emerges from the expansion (3.7) as a Weyl-ordered series. Conversely, if the operator $\hat{O}(\hat{r},\hat{k})$ is given by a Weyl-ordered power series

$$\hat{O}(\hat{r},\hat{k})=\sum_{\substack{m_1,m_2,m_3\\ n_1,n_2,n_3}}A_{n_1,n_2,n_3}^{m_1,m_2,m_3}\{\hat{r}_1^{m_1}\hat{r}_2^{m_2}\hat{r}_3^{m_3}\hat{k}_1^{n_1}\hat{k}_2^{n_2}\hat{k}_3^{n_3}\}_W\ , \tag{3.8}$$

then by choosing in (3.7) the $O(r,k)$

$$O(r,k)=\sum_{\substack{m_1,m_2,m_3\\ n_1,n_2,n_3}}A_{n_1,n_2,n_3}^{m_1,m_2,m_3}r_1^{m_1}r_2^{m_2}r_3^{m_3}k_1^{n_1}k_2^{n_2}k_3^{n_3} \tag{3.9}$$

formally reproduces the series (3.8). Like the ordinary Weyl transform in (1.5) and (1.6), the Weyl transform of the Weyl-ordered function $\hat{O}(\hat{r},\hat{k})$ is obtained by replacing the operators $\hat{r},\hat{k}$ with the $c$ numbers $r,k$.

If the operator $\hat{O}(\hat{r},\hat{k})$ is expressed in some other ordering than the Weyl order, its Weyl transform may still be found from (3.6). In principle one might also recast the operator into Weyl order and then replace $\hat{r},\hat{k}$ with $r,k$. We give here an example that demonstrates the salient difference from the ordinary Weyl transform. In contrast to $\hat{p}_i$, different components of the kinetic momentum $\hat{k}$ in general do not commute, and from (2.15) we obtain

$$\hat{k}_1\hat{k}_2=\tfrac{1}{2}[\hat{k}_1\hat{k}_2+\hat{k}_2\hat{k}_1]+i\frac{\hbar Q}{2}\hat{B}_3(\hat{r})\leftrightarrow k_1k_2+i\frac{\hbar Q}{2}B_3(r)\ . \tag{3.10}$$

The appearance of the magnetic field in the commutators of $\hat{k}_i$ does not cause any conceptual problems in the case of the classical field, but it is going to introduce essential complications when the EM field is quantized; see Secs. III B and IV.

From (3.5) and (2.18) it follows that the quantum-mechanical expectation value of $\hat{O}$ can again be calculated as if the Weyl transform $O$ were a classical function whose average is obtained using the "phase-space density" $W$,

$$\mathrm{Tr}(\hat{O}\hat{\rho})=\int d^3r\, d^3k\, O(r,k)W(r,k)\ . \tag{3.11}$$

The GIWF is real, but because it contains the ordinary WF as a special case (with $\hat{A}=0$), it cannot be guaranteed to be non-negative.

To complete the program patterned in the Introduction an equation of motion for the GIWF is needed. This we derive in Secs. IV and V. For the time being we turn to a discussion of gauge independence and gauge invariance in our formulation.

### 1. Gauge invariance with classical fields

The gauge transformation[31]

$$\hat{A}(\hat{r},t)\to\hat{A}'(\hat{r},t)=\hat{A}(\hat{r},t)+\frac{\partial}{\partial\hat{r}}\hat{\chi}(\hat{r},t)\ , \tag{3.12a}$$

$$\hat{\Phi}(\hat{r},t)\to\hat{\Phi}'(\hat{r},t)=\hat{\Phi}(\hat{r},t)-\frac{\partial}{\partial t}\hat{\chi}(\hat{r},t)\ , \tag{3.12b}$$

generated by an arbitrary real function $\chi(r,t)$ leaves the physical fields unchanged. In order to keep the Schrödinger equation form invariant under the gauge transformation, it is postulated that a simultaneous unitary transformation defined by the operator

$$\hat{G}=\exp\left[\frac{iQ}{\hbar}\hat{\chi}(\hat{r},t)\right] \tag{3.13}$$

must be effected on the states and operators characterizing the quantum system. The vectors of the Hilbert space transform according to

$$|\Psi\rangle\to|\Psi'\rangle=\hat{G}|\Psi\rangle\ , \tag{3.14}$$

and the operators, including the density operator $\hat{\rho}$, become

$$\hat{O}\to\hat{O}'=\hat{G}\hat{O}\hat{G}^\dagger\ . \tag{3.15}$$

Let us now study the operator

$$\hat{O}=O(\hat{r},\hat{p};\hat{A}(\hat{r},t),\hat{\Phi}(\hat{r},t);\{\hat{E}(\hat{r},t),\hat{B}(\hat{r},t)\};t) \tag{3.16}$$

that depends explicitly on the electromagnetic potentials $\hat{A}$ and $\hat{\Phi}$, and also in some uniquely prescribed functional manner on the physical fields $\hat{E}$ and $\hat{B}$. Such an operator is called gauge invariant if it retains its form under a gauge transformation,

$$\hat{O}(\hat{r},\hat{p};\hat{A},\hat{\Phi})\to\hat{O}'=\hat{G}\hat{O}\hat{G}^\dagger=\hat{O}(\hat{r},\hat{p};\hat{A}',\hat{\Phi}')\ . \tag{3.17}$$

It may be postulated that *only gauge-invariant operators represent observable physical quantities.*[31] From the point of view of practical calculations a gauge-invariant operator possesses the advantage that its form in any gauge is known and does not depend on the arbitrary function $\chi$, hence the actual expression of $\hat{O}$ is also immediately known in any fixed gauge.

It is well known that the kinetic momentum $\hat{k}$ is a gauge-invariant operator, whereas the canonical momentum $\hat{p}$ is not. It follows that every operator $\hat{O}(\hat{r},\hat{p};\hat{A},\hat{\Phi})$ that depends on the potentials only through the combination $\hat{k}=\hat{p}-Q\hat{A}$ is gauge invariant. Although it seems to be difficult to formulate the proof, we conjecture that the inverse of this statement also holds: By reordering the operators all gauge-independent operators may be cast into the form

$$\hat{O}=\hat{O}(\hat{r},\hat{k};\{\hat{E}(\hat{r},t),\hat{B}(\hat{r},t)\}) , \tag{3.18}$$

which may contain a functional dependence on the physical fields $\hat{E}$ and $\hat{B}$.

Since the GIWO (2.17) is a function of $\hat{r}$ and $\hat{k}$ only, it is a gauge-invariant operator. Hence its explicit form in any gauge is known. If the density operator is known (in the same gauge), the GIWF may be calculated. Furthermore, being a quantum-mechanical expectation value independent of the unitary transformation [(3.13)–(3.15)], the GIWF actually is *independent* of the gauge. The potential $\hat{A}$ only appears as an auxiliary device during the calculations.

However, the quantum-mechanical state $\hat{\rho}$ for a system needed to obtain the GIWF is *a priori* known only by assumption. For instance, thermal equilibrium may be assumed if $\hat{E}=0$ and $\hat{B}$ is time independent. If a process of preparation or measurement is needed to determine the state, the problem of relating the gauge-independent measured values to the state remains, cf. Ref. 17. In earlier investigations of gauge invariance[16,18,31,32] the problem is partly concealed by stating that in an experiment transitions between (in general, time dependent) eigenstates of some gauge-invariant operator are observed, and the gauge-independent transition amplitudes are sufficient to describe the experiment. In effect, the conventional approach *assumes* that the initial state of the system *is known.*

The GIWF provides a handy solution to relating the state of the system to measurements. To see this, we formulate another postulate: *Expectation values of gauge-invariant operators can be measured without ever having to refer to the gauge of the EM field.* For each fixed $r,k$ the GIWO is a gauge-invariant Hermitian operator, hence one can (in principle) measure its expectation value, $W(r,k)$, without invoking the gauge. In an ensemble of identical systems this can (in principle?) be repeated for every $r,k$, and the whole GIWF $W(r,k)$ is determined. That is, "the state" of the system can be measured.

According to (3.17) the gauge transformation of any gauge-invariant operator is a unitary transformation. Since traces are preserved in unitary transformations, it follows immediately from the definition (3.6) that the Weyl transform $O(r,k)$ of any gauge-invariant operator $\hat{O}$ is gauge independent.

Suppose the GIWF $W(r,k,t_0)$ is initially determined either by a measurement or an assumption. Next the system is allowed to evolve and at time $t$ the expectation value of some gauge-invariant operator $\hat{O}$ is measured. The result is

$$\mathrm{Tr}[\hat{\rho}(t)\hat{O}]=\int d^3r\,d^3k\,O(r,k)W(r,k,t) .$$

It will be shown in Sec. V that the equation of motion of the GIWF only involves the physical fields $E,B$. We have thus provided a full quantum-mechanical description of an experimental run, where the gauge fields at most appear as auxiliary devices in calculations. We note that a third way to determine the initial density matrix is to *prepare* the system in some chosen state. This may also be expressed in terms of the GIWF, but a closer investigation of this aspect will be the subject of a separate publication.[33]

### B. The case of quantized field modes

When quantized modes of the EM field are present, $\hat{A}(\hat{r},t)$ [and possibly $\hat{\Phi}(\hat{r},t)$] are operators also in the degrees of freedom of the EM field. The vectors $|r\rangle$ (or $|p\rangle$) no longer form a complete basis of the quantum-mechanical part of the problem. Instead, one must use as a basis either the vectors

$$|r,\lambda\rangle=|r\rangle|\lambda\rangle , \tag{3.19}$$

where $\lambda$ enumerates the vectors in some basis of the quantized field, or any other basis obtained from the tensor products in (3.19) by means of a unitary transformation.

In nonrelativistic quantum electrodynamics problems of reconciling gauge transformations and quantization of the field are usually avoided by using the Coulomb gauge and quantizing only the transverse part of the EM field. Here we adhere to the same procedure. The vector potential $\hat{A}_Q(\hat{r})$ is quantized, but the scalar potential $\Phi(\hat{r},t)$ is still an operator only via its argument $\hat{r}$.

The BCH formulas (2.25)–(2.27) remain valid when quantized fields are present. By using the forms (2.25a) and (2.25c) in the product of the operators and by taking the partial trace with respect to the particle's degrees of freedom, we obtain analogously to (3.4) the result

$$\mathrm{Tr}_P[\hat{W}(r,k)\hat{W}(r',k')]=(2\pi\hbar)^{-3}\delta(r-r')\delta(k-k')1_F , \tag{3.20}$$

where $1_F$ stands for the unit operator in the field degrees of freedom.

For the case of quantized fields the set of operators for the system particle + field is much larger than for a classical field; functions of the boson operators $\hat{b}_q,\hat{b}_q^\dagger$ are also incorporated. The GIWF is useful only if one finds for a sufficiently large class of operators $\hat{O}$ the Weyl transform $O(r,k)$ satisfying

$$\mathrm{Tr}(\hat{O}\hat{\rho})=\int d^3r\,d^3k\,O(r,k)W(r,k) . \tag{3.21}$$

We first note that (3.21) trivially holds for any operator $\hat{O}$ that can be represented in the form

$$\hat{O}(\hat{r},\hat{k})=\int d^3r\,d^3k\,O(r,k)\hat{W}(r,k)\ , \quad (3.22)$$

with $O(r,k)$ being a $c$-number function. As argued previously, an expansion of (3.22) in the form (3.7) gives a Weyl-ordered series in $\hat{r}$ and $\hat{k}$. Conversely, if $\hat{O}(\hat{r},\hat{k})$ is given by a Weyl-ordered series of $\hat{r}$ and $\hat{k}$, the representation (3.22) results by simply using inside the integral the function $O(r,k)$ obtained from $\hat{O}(\hat{r},\hat{k})$ through the replacement $\hat{r},\hat{k}\rightarrow r,k$. If it is not known whether the expansion (3.22) is possible, the necessary condition from (3.20) and (3.22),

$$\mathrm{Tr}_P[\hat{O}\hat{W}(r,k)]=(2\pi\hbar)^{-3}O(r,k)\mathbf{1}_F\propto\mathbf{1}_F \quad (3.23)$$

may supply at least the negative answer.

In conclusion, we have argued that for a Weyl-ordered operator $\hat{O}(\hat{r},\hat{k})$ one expects to find the "Weyl transform" $O(r,k)$ satisfying (3.21) and (3.22). What happens if $\hat{O}$ is not Weyl ordered can be appreciated in an example derived from (3.10):

$$\mathrm{Tr}(\hat{k}_1\hat{k}_2\hat{\rho})=\int d^3r\,d^3k\,k_1k_2W(r,k)+\frac{i\hbar Q}{2}\mathrm{Tr}[\hat{B}_3(\hat{r})\hat{\rho}]\ . \quad (3.24)$$

If $\hat{Q}$ is not Weyl ordered, the form (3.21) is in general possible only if also the expectation values of (products of derivatives of) the magnetic field can be expressed in that form. At first glance one might argue that by taking the trace in the definition of the GIWF (2.18), one loses too much information about the electromagnetic field, so such expectation values could no longer be retrieved. But we have not been able to prove this, and the contrary may hold. In fact, the radiation-reaction fields can sometimes be expressed in terms of the operator $\hat{k}$, thus some of their moments may be deduced from the GIWF.[20]

## IV. EQUATION OF MOTION FOR THE WIGNER OPERATOR

### A. The Heisenberg picture

We now embark on a study of the dynamical properties of the system charged particle + field. The time evolution is generated by the Hamiltonian

$$\hat{H}=\sum_i\frac{\hat{k}_i(t)\hat{k}_i(t)}{2M}+Q\hat{\Phi}(\hat{r},t)+\hbar{\sum_q}'\Omega_q\hat{b}_q^\dagger\hat{b}_q\ . \quad (4.1)$$

The first term is the kinetic energy, the second is the scalar potential of the EM field, and the third is the free-field Hamiltonian. If present, any potential of nonelectromagnetic origin may be added to $Q\hat{\Phi}$ and treated precisely in the same way as this. We allow both for external classical time-dependent fields $\hat{A}_C$, $\hat{\Phi}$, and the quantized field $\hat{A}_Q$ which is time independent in the Schrödinger picture. The unitary time-evolution operator of the system $\hat{U}(t,t_0)$ satisfies the equations

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)=\hat{H}(t)\hat{U}(t,t_0)\ , \quad (4.2a)$$

$$\hat{U}(t_0,t_0)=1\ . \quad (4.2b)$$

Given the density operator $\hat{\rho}(t_0)$ at time $t_0$, at time $t$ it is

$$\hat{\rho}(t)=\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)\ . \quad (4.3)$$

The transformation of the operator

$$\hat{O}(t)=\hat{O}(\hat{r},\hat{p},\{\hat{b}_q\},\{\hat{b}_q^\dagger\};t) \quad (4.4)$$

to the Heisenberg picture is defined by

$$\hat{O}_H(t)=\hat{U}^\dagger(t,t_0)\hat{O}(t)\hat{U}(t,t_0)\ . \quad (4.5)$$

$\hat{O}_H$ is the same function of the operators as (4.4), except that $\hat{r},\hat{p}$, etc., are replaced with their Heisenberg transforms. Notice that the time-evolution operator is unitary, hence the commutators of the operators are preserved in the Heisenberg picture. It follows from (4.2a) and its Hermitian conjugate that

$$\frac{d}{dt}\hat{O}_H(t)=-\frac{i}{\hbar}[\hat{O}_H(t),\hat{H}_H(t)]+\frac{\partial}{\partial t}\hat{O}_H(t)\ , \quad (4.6)$$

where $\partial/\partial t$ stands for the partial derivative with respect to the explicit time dependence of the operator function (4.4).

Along the lines of (3.5) and (3.21) we now assume that in the Schrödinger picture an operator $\hat{O}(t)$ can be represented in the form

$$\hat{O}(t)=\int d^3r\,d^3k\,O(r,k,t)\hat{W}(r,k;\hat{r},\hat{k}(t))\ , \quad (4.7)$$

where $O(t)$ is the Weyl transform of $\hat{O}(t)$ at time $t$. Then, at time $t$ the expectation value of the operator $\hat{O}(t)$ is

$$\mathrm{Tr}[\hat{O}(t)\hat{\rho}(t)]=\int d^3r\,d^3k\,O(r,k,t)\mathrm{Tr}[\hat{W}(t)\hat{U}(t,t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t,t_0)]=\int d^3r\,d^3k\,O(r,k,t)\mathrm{Tr}[\hat{W}_H(t)\hat{\rho}(t_0)]\ . \quad (4.8)$$

We therefore use the Heisenberg-picture expectation value of the GIWO,

$$W(r,k,t)=\mathrm{Tr}[\hat{W}_H(r,k,t)\hat{\rho}(t_0)]\ , \quad (4.9)$$

as the time-dependent generalization of the GIWF.

We have now carefully defined the Heisenberg picture in the case when both the Hamiltonian and the operators considered depend explicitly on time. The strategy of our subsequent considerations is the following. First we derive the Heisenberg equation of motion for the GIWO $\hat{W}_H$. Next, we assume that quantized fields are absent, multiply the Heisenberg equation of motion with $\hat{\rho}(t_0)$, and take the trace. This gives a closed equation for the GIWF. The expectation values of any operators that can be presented in the form (4.7), e.g., of any Weyl-ordered function of $\hat{r}$ and $\hat{k}$, may then be calculated. We note that a closed equation can be derived for the GIWF also when radiation-reaction fields are present; this is the main theme of the second paper in this series.[20]

### B. Heisenberg equation of motion

In this section we derive the Heisenberg equation of motion for the Wigner operator $\hat{W}_H$. Since we use the Heisenberg picture throughout the rest of this paper, the subscript $H$ will often be omitted in the operators. As the transformation to the Heisenberg picture preserves commutators, at every instant of time it is possible to find a temporary basis $\{|r,\lambda\rangle\}$ consisting of the eigenstates of $\hat{r}(t)$ and satisfying

$$\hat{r}\,|r,\lambda\rangle \equiv \hat{r}_H(t)\,|r,\lambda\rangle = r\,|r,\lambda\rangle \ , \tag{4.10a}$$

$$\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]|r,\lambda\rangle = |r-u,\lambda\rangle \ , \tag{4.10b}$$

$$\langle r,\lambda\,|\,\hat{O}(\hat{r};\{\hat{b}_q\},\{\hat{b}_q^\dagger\})\,|\,r',\lambda'\rangle = \langle r,\lambda\,|\,\hat{O}(r;\{\hat{b}_q\},\{\hat{b}_q^\dagger\})\,|\,r',\lambda'\rangle \ . \tag{4.10c}$$

Here $\lambda$ labels some quantum numbers other than $r$ needed to specify the state uniquely. For instance, the basis obtained from the one in (3.19) via the transformation

$$|r,\lambda\rangle = \hat{U}(t,t_0)\,|r\rangle\,|\lambda\rangle \tag{4.11}$$

satisfies (4.10). Similarly, all operator equations that follow from the commutators, in particular (2.19b) and (2.25)–(2.27), remain valid in the Heisenberg picture.

The task is to calculate

$$\frac{d}{dt}\hat{W}(r,k;\hat{r},\hat{k}(t)) = \frac{\partial}{\partial t}\hat{W}(r,k;\hat{r},\hat{k}(t)) - \frac{i}{\hbar}\left[\hat{W}(r,k;\hat{r},\hat{k}(t)),\sum_i\frac{\hat{k}_i(t)\hat{k}_i(t)}{2M} + Q\hat{\Phi}(\hat{r},t) + \hbar{\sum_q}'\Omega_q\hat{b}_q^\dagger\hat{b}_q\right] , \tag{4.12}$$

where the explicit time dependence has been indicated (below this is done only when the time dependence is specifically emphasized). $\hat{W}$ is given by

$$\hat{W}(r,k) = \frac{1}{(2\pi\hbar)^6}\int d^3u\,d^3v\,\exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right]\hat{T}(u,v) \ ,$$

$$\hat{T}(u,v) = \exp\left[\frac{i}{\hbar}(u\cdot\hat{k}+v\cdot\hat{r})\right] = \exp\left[\frac{i}{\hbar}(v\cdot\hat{r}+u\cdot\{\hat{p}-Q[\hat{A}_C(\hat{r},t)+\hat{A}_Q(\hat{r})]\})\right] .$$

We start with the contribution to the equation of motion owing to the commutator with the scalar potential. Using (2.25c) and (2.19b) we obtain

$$(2\pi\hbar)^6\left[-\frac{iQ}{\hbar}\right][\hat{W}(r,k),\hat{\Phi}(\hat{r},t)] = -\frac{iQ}{\hbar}\int d^3u\,d^3v\left\{\exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r-\tfrac{1}{2}u\cdot v)\right]\exp\left[\frac{i}{\hbar}\left[v\cdot\hat{r}-Qu\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}+\tau u)\right]\right]\right.$$
$$\left.\times[\hat{\Phi}(\hat{r}+u)-\hat{\Phi}(\hat{r})]\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]\right\} . \tag{4.13}$$

We now write

$$\hat{\Phi}(\hat{r}+u)-\hat{\Phi}(\hat{r}) = u\cdot\int_0^1 d\tau\left[\frac{\partial\hat{\Phi}}{\partial\hat{r}}\right](\hat{r}+\tau u) \ . \tag{4.14}$$

The special notation inside the integral stands for the derivative of $\hat{\Phi}$ with respect to $\hat{r}$ taken at the point $\hat{r}+\tau u$. In the sequel we adhere to this convention in order to distinguish *functions* that are formed by taking derivatives from *objects acted on* by the derivative operator. Unless otherwise stated, below the operator $\partial/\partial k$ $(\partial/\partial r)$ acts on all $k$ $(r)$ dependence on the right of it.

Next we take the matrix element of (4.13) between two states of the temporary basis. From (4.10b) and (4.10c) we obtain

$$(2\pi\hbar)^6\left[-\frac{iQ}{\hbar}\right]\langle r',\lambda'\,|\,[\hat{W}(r,k),\hat{\Phi}(\hat{r},t)]\,|\,r'',\lambda''\rangle$$
$$= -\frac{iQ}{\hbar}\int d^3u\,d^3v\left\{\exp\left[-\frac{i}{\hbar}(u\cdot k+v\cdot r-\tfrac{1}{2}u\cdot v)\right]\exp\left[\frac{i}{\hbar}v\cdot r'\right]u\cdot\int_0^1 d\tau\left[\frac{\partial\Phi}{\partial r}\right](r'+\tau u)\right.$$
$$\left.\times\left\langle r',\lambda'\left|\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(r'+\tau u)\right]\right|r''-u,\lambda''\right\rangle\right\} . \tag{4.15a}$$

The integral over $v$ could now be carried out, and it would give a result proportional to $\delta[r'-(r-\frac{1}{2}u)]$. It can thus be seen that all matrix elements (4.15a) remain unchanged, if the replacement

$$\left[\frac{\partial\Phi}{\partial r}\right](r'+\tau u)\rightarrow\left[\frac{\partial\Phi}{\partial r}\right](r-\tfrac{1}{2}u+\tau u) \tag{4.15b}$$

is carried out. Hence we may from (4.15) restore the operator equation

$$-\frac{iQ}{\hbar}[\hat{W}(r,k),\Phi(\hat{r},t)]=\frac{-iQ}{\hbar(2\pi\hbar)^6}\int d^3u\,d^3v\left\{u\cdot\int_{-1/2}^{1/2}d\tau\left[\frac{\partial\Phi}{\partial r}\right](r+\tau u)\right\}\exp\left\{-\frac{i}{\hbar}(u\cdot k+v\cdot r)\right\}\hat{T}(u,v)\;. \tag{4.16}$$

We may finally bring the function of $u$ appearing inside the first set of large parentheses outside the integral by replacing each $u$ with $-(\hbar/i)(\partial/\partial k)$,

$$-\frac{iQ}{\hbar}[\hat{W}(r,k),\hat{\Phi}(\hat{r},t)]=Q\frac{\partial}{\partial k}\cdot\int_{-1/2}^{1/2}d\tau\left[\frac{\partial\Phi}{\partial r}\right]\left\{r+i\hbar\tau\frac{\partial}{\partial k}\right\}\hat{W}(r,k)\;. \tag{4.17}$$

It can be seen right away that this operator term is precisely of the same form as the potential term in the equation of motion of the ordinary WF, (1.11).

Steps very similar to the ones carried out above give the explicit time derivative in the form

$$\left[\frac{\partial\hat{W}}{\partial t}\right](r,k,t)=Q\frac{\partial}{\partial k}\cdot\int_{-1/2}^{1/2}d\tau\left[\frac{\partial A_C}{\partial t}\right]\left\{r+i\hbar\tau\frac{\partial}{\partial k},t\right\}\hat{W}(r,k,t)\;. \tag{4.18}$$

We next focus on the commutator with the free-field Hamiltonian in (4.12). We begin with

$$[\hat{T}(u,v),\hat{b}_q^\dagger\hat{b}_q]=\exp\left[\frac{i}{\hbar}\left[\tfrac{1}{2}u\cdot v+v\cdot\hat{r}-Qu\cdot\int_0^1 d\tau\,\hat{A}_C(\hat{r}+\tau u,t)\right]\right]$$
$$\times\left[\exp\left\{-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}_Q(\hat{r}+\tau u)\right\},\hat{b}_q^\dagger\hat{b}_q\right]\exp\left\{\frac{i}{\hbar}u\cdot\hat{p}\right\}\;. \tag{4.19}$$

From (2.4) we obtain

$$-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}_Q(\hat{r}+\tau u)=-i\sum_q{}'(\hat{a}_q\hat{b}_q^\dagger+\hat{a}_q^\dagger\hat{b}_q)\;, \tag{4.20a}$$

with

$$\hat{a}_q=\frac{iQ}{\hbar}u\cdot g(q)\int_0^1 d\tau\exp[-iq\cdot(\hat{r}+\tau u)]\;. \tag{4.20b}$$

Because $\hat{a}_q,\hat{a}_q^\dagger$ commute with each other and with the field operators, and the field operators of different modes also commute with each other, the commutator in (4.19) may be obtained explicitly:

$$[\;,\;]=\exp\left\{-\sum_{q'\neq q}{}'(\hat{a}_{q'}\hat{b}_{q'}^\dagger+\hat{a}_{q'}^\dagger\hat{b}_{q'})\right\}[\exp[-i(\hat{a}_q\hat{b}_q^\dagger+\hat{a}_q^\dagger\hat{b}_q)],\hat{b}_q^\dagger\hat{b}_q]$$
$$=i\left[\hat{a}_q\hat{b}_q^\dagger\exp\left\{-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}_Q(\hat{r}+\tau u)\right\}-\exp\left\{-\frac{iQ}{\hbar}u\cdot\int_0^1 dt\,\hat{A}_Q(\hat{r}+\tau u)\right\}\hat{a}_q^\dagger\hat{b}_q\right]\;. \tag{4.21}$$

Comparing (4.20b) and the definitions of the field operators $\hat{E}_Q^{(\pm)}$, (2.11), we have the result

$$-\frac{i}{\hbar}\left[\hat{T}(u,v),\hbar\sum_q{}'\hat{b}_q^\dagger\hat{b}_q\right]$$
$$=\frac{iQ}{\hbar}\exp\left\{\frac{i}{\hbar}(\tfrac{1}{2}u\cdot v+v\cdot\hat{r})\right\}\left[u\cdot\int_0^1 d\tau\,\hat{E}_Q^{(-)}(\hat{r}+\tau u)\exp\left\{-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}+\tau u)\right\}\right.$$
$$\left.+\exp\left\{-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}+\tau u)\right\}u\cdot\int_0^1 d\tau\,\hat{E}_Q^{(+)}(\hat{r}+\tau u)\right]\exp\left\{\frac{i}{\hbar}u\cdot\hat{p}\right\}\;. \tag{4.22}$$

The steps just like those from (4.13) to (4.17) finally give

$$-\frac{i}{\hbar}\left[\hat{W}(r,k),\hbar\sum_q{}'\Omega_q\hat{b}_q^\dagger\hat{b}_q\right]=-Q\frac{\partial}{\partial k}\cdot\left[\int_{-1/2}^{1/2}d\tau\hat{E}_Q^{(-)}\left[r+i\hbar\tau\frac{\partial}{\partial k}\right]\hat{W}(r,k)+\hat{W}(r,k)\int_{-1/2}^{1/2}d\tau\hat{E}_Q^{(+)}\left[r+i\hbar\tau\frac{\overleftarrow{\partial}}{\partial k}\right]\right]. \quad (4.23)$$

In this equation $\hat{E}_Q^{(\pm)}$ are still operators on the EM degrees of freedom, and therefore the order of $\hat{E}_Q^{(\pm)}$ and $\hat{W}$ need to be specified. Notice that the negative- (positive-) frequency component of the electric field appears to the left (right) of the GIWO. The arrow above one of the derivatives indicates that this derivative exceptionally acts to the left.

The evaluation of the remaining commutator involving the kinetic energy in the equation of motion (4.12) is quite a laborous task. We do not present it in all detail, but only give an outline and derive some auxiliary results. Our tactic is to keep the operator $\hat{k}=\hat{p}-Q\hat{A}(\hat{r})$ unsplit as far as possible. Therefore we employ the BCH formula (2.26a).

For the time being we, however, split $\exp[(i/\hbar)u\cdot\hat{k}]$ according to (2.27a), and obtain the commutator

$$\left[\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right],\hat{k}_i\right]=\left[\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\hat{A}(\hat{r}+\tau u)\right],\hat{p}_i\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]-Q\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\hat{A}(\hat{r}+\tau u)\right]\left[\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right],\hat{A}_i(\hat{r})\right]. \quad (4.24)$$

In spite of the fact that $\hat{A}(\hat{r})$ may contain quantum-field operators, (2.5) ensures that in operator formulas involving only functions of $\hat{r}$, $\hat{p}$, and $\hat{A}(\hat{r})$ and its spatial derivatives, the quantum-field nature never shows explicitly. Consequently, the textbook result

$$[\hat{f}(\hat{r}),\hat{p}_i]=i\hbar\left[\frac{\partial\hat{f}}{\partial\hat{r}_i}\right](\hat{r})$$

still applies to the first commutator on the right-hand side of (4.24), whereas the second follows from (2.19b). We obtain from (4.24)

$$\begin{aligned}\left[\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right],\hat{k}_i\right]&=Q\left[\sum_j u_j\int_0^1 d\tau\left[\frac{\partial\hat{A}_j}{\partial\hat{r}_i}\right](\hat{r}+\tau u)-[\hat{A}_i(\hat{r}+\tau u)-\hat{A}_i(\hat{r})]\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]\\&=Q\sum_j u_j\left[\int_0^1 d\tau\left[\frac{\partial\hat{A}_j}{\partial\hat{r}_i}\right](\hat{r}+\tau u)-\int_0^1 d\tau\left[\frac{\partial\hat{A}_i}{\partial\hat{r}_j}\right](\hat{r}+\tau u)\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]\\&=Q\int_0^1 d\tau\left[u\times\left[\frac{\partial}{\partial r}\times\hat{A}\right](\hat{r}+\tau u)\right]_i\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]\\&=Q\int_0^1 d\tau\{u\times\hat{B}(\hat{r}+\tau u)\}_i\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right],\end{aligned} \quad (4.25)$$

where we have used a standard formula of vector analysis derived from

$$\sum_k \epsilon_{ijk}\epsilon_{i'j'k}=\delta_{ii'}\delta_{jj'}-\delta_{ij'}\delta_{i'j}.$$

It is also immediately obvious that

$$\left[\exp\left[\frac{i}{\hbar}v\cdot\hat{r}\right],\hat{k}_i\right]=-v_i\exp\left[\frac{i}{\hbar}v\cdot\hat{r}\right]. \quad (4.26)$$

It follows from (2.26a), (4.25), and (4.26) that

$$[\hat{T}(u,v),\hat{k}_i\hat{k}_i]=\exp\left[\frac{i}{\hbar}(\tfrac{1}{2}u\cdot v+v\cdot\hat{r})\right]\left[Q\left[-i\hbar\frac{\partial}{\partial\hat{r}_i}+Q\int_0^1 d\tau[u\times\hat{B}(\hat{r}+\tau u)]_i\right]\int_0^1 d\tau[u\times\hat{B}(\hat{r}+\tau u)]_i + 2Q\int_0^1 d\tau[u\times\hat{B}(\hat{r}+\tau u)]_i\hat{k}_i - v_i(v_i+2\hat{k}_i)\right]\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]. \qquad (4.27)$$

It pays to remove the product $\hat{k}_i\exp[(i/\hbar)u\cdot\hat{k}]$ from (4.27). To this end we first take the derivative of (2.27b) with respect to $u_i$, and obtain

$$\frac{\partial}{\partial u_i}\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]=\frac{i}{\hbar}\exp\left[\frac{i}{\hbar}u\cdot\hat{p}\right]\left[\hat{p}_i-Q\int_0^1 d\tau\,\hat{A}_i(\hat{r}-\tau u)+Q\sum_j u_j\int_0^1 d\tau\,\tau\left[\frac{\partial\hat{A}_j}{\partial\hat{r}_i}\right](\hat{r}-\tau u)\right]\times\exp\left[-\frac{iQ}{\hbar}u\cdot\int_0^1 d\tau\,\hat{A}(\hat{r}-\tau u)\right]. \qquad (4.28)$$

From the simple equality

$$\frac{\partial}{\partial\tau}[\tau\hat{A}_i(\hat{r}-\tau u)]=\hat{A}_i(\hat{r}-\tau u)-\tau\sum_j u_j\left[\frac{\partial\hat{A}_i}{\partial\hat{r}_j}\right](\hat{r}-\tau u) \qquad (4.29a)$$

it follows by integration that

$$\int_0^1 d\tau\,\hat{A}_i(\hat{r}-\tau u)=\hat{A}_i(\hat{r}-\tau u)+\sum_j u_j\int_0^1 d\tau\,\tau\left[\frac{\partial\hat{A}_i}{\partial\hat{r}_j}\right](\hat{r}-\tau u). \qquad (4.29b)$$

When (4.29b) is inserted into (4.28), just as in (4.25) the derivatives again combine to give the magnetic field. With the aid of (2.19b), (4.28) becomes

$$\frac{\partial}{\partial u_i}\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]=\frac{i}{\hbar}\left[\hat{k}_i+Q\int_0^1 d\tau(1-\tau)[u\times\hat{B}(\hat{r}+\tau u)]_i\right]\times\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right], \qquad (4.30a)$$

or equivalently,

$$\hat{k}_i\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]=\left[\frac{\hbar}{i}\frac{\partial}{\partial u_i}-Q\int_0^1 d\tau(1-\tau)[u\times\hat{B}(\hat{r}+\tau u)]_i\right]\times\exp\left[\frac{i}{\hbar}u\cdot\hat{k}\right]. \qquad (4.30b)$$

This expression was derived here because it shows a way to handle products involving the GIWO and the operator $\hat{k}$; an application is presented elsewhere.[20]

The derivation proceeds as follows. First (4.30b) is inserted into (4.27). Next the Fourier transform $\hat{T}(u,v)\to\hat{W}(r,k)$ is introduced. By several partial integrations and steps like those from (4.13) to (4.17) the desired commutator is finally obtained.

We collect all terms in (4.12) and write the complete equation of motion for the GIWO:

$$\left[\frac{\partial}{\partial t}+\tilde{v}\cdot\frac{\partial}{\partial r}+Q\frac{\partial}{\partial k}\cdot[\tilde{v}\times\tilde{B}+\tilde{E}_C]\right]\hat{W}(r,k,t)+Q\frac{\partial}{\partial k}\cdot\left[\tilde{E}_Q^{(-)}\hat{W}(r,k,t)+\hat{W}(r,k,t)\tilde{E}_Q^{(+)}\right]=0. \qquad (4.31)$$

Here the symbols marked with tildes may be operators in the quantum-field degrees of freedom, and because they contain powers of $\partial/\partial k$ that operate on the label $k$ of the GIWO, we have

$$\tilde{v}=v+\Delta\tilde{v}=\frac{k}{M}-\frac{Q}{M}\frac{\hbar}{i}\frac{\partial}{\partial k}\times\int_{-1/2}^{1/2}d\tau\,\tau\hat{B}\left[r+i\hbar\tau\frac{\partial}{\partial k}\right], \qquad (4.32a)$$

$$\tilde{B}=\int_{-1/2}^{1/2}d\tau\,\hat{B}\left[r+i\hbar\tau\frac{\partial}{\partial k}\right], \qquad (4.32b)$$

$$\tilde{E}_C=\int_{-1/2}^{1/2}d\tau\left\{-\left[\frac{\partial\Phi}{\partial r}\right]\left[r+i\hbar\tau\frac{\partial}{\partial k}\right]-\left[\frac{\partial A_C}{\partial t}\right]\left[r+i\hbar\tau\frac{\partial}{\partial k}\right]\right\}=\int_{-1/2}^{1/2}E_C\left[r+i\hbar\tau\frac{\partial}{\partial k}\right], \qquad (4.32c)$$

$$\tilde{E}_Q^{(\pm)}=\int_{-1/2}^{1/2}d\tau\,\hat{E}_Q^{(\pm)}\left[r+i\hbar\tau\frac{\overleftrightarrow{\partial}}{\partial k}\right]. \qquad (4.32d)$$

Note that in the last term of (4.31) the derivatives inside $\hat{E}^{(+)}$ exceptionally act to the left.

Qualitatively this equation of motion mimics the equation of motion for the phase-space density of a particle subjected to the Lorentz force $Q(v\times B+E)$. Quantum mechanics appear in the field-operator character of $\tilde{B}$, $\tilde{E}_Q^{(\pm)}$, and $\hat{W}$, in the "normal" ordering of $\tilde{E}_Q^{(\pm)}$ and $\hat{W}$, and in the operator arguments $i\hbar\tau(\partial/\partial k)$ of the fields. Only one real surprise is present, namely, the velocity correction

$$\Delta\tilde{v}=-\frac{Q}{M}\frac{\hbar}{i}\frac{\partial}{\partial k}\times\int_{-1/2}^{1/2}d\tau\,\tau\hat{B}\left[r+i\hbar\tau\frac{\partial}{\partial k}\right],$$

which always adds to the ordinary velocity $k/M$. This is a genuine quantum feature, at least of the order $\hbar^2$, but otherwise we have no physical explanation to offer.

## V. EQUATION OF MOTION FOR FULLY CLASSICAL FIELDS

When only a classical field is present, one immediately obtains the equation of motion for the GIWF by multiplying (4.31) by $\hat{\rho}(t_0)$ and taking the trace. To allow a closer examination we write the result using the position and velocity variables $r$ and $v=k/M$,

$$\left[\frac{\partial}{\partial t}+(v+\Delta\tilde{v})\cdot\frac{\partial}{\partial r}+\frac{Q}{M}\frac{\partial}{\partial v}\cdot[(v+\Delta\tilde{v})\times\tilde{B}+\tilde{E}]\right]W(r,v,t)=0 \quad (5.1)$$

with

$$\Delta\tilde{v}=-\frac{Q}{M^2}\frac{\hbar}{i}\frac{\partial}{\partial v}\times\int_{-1/2}^{1/2}d\tau\,\tau B\left[r+\frac{i\hbar\tau}{M}\frac{\partial}{\partial v}\right], \quad (5.2a)$$

$$\tilde{B}=\int_{-1/2}^{1/2}d\tau\,B\left[r+\frac{i\hbar\tau}{M}\frac{\partial}{\partial v}\right],$$

$$\tilde{E}=\int_{-1/2}^{1/2}d\tau\,E\left[r+\frac{i\hbar\tau}{M}\frac{\partial}{\partial v}\right]. \quad (5.2b)$$

In the limit $\hbar\to 0$ (5.1) and (5.2) give precisely the classical Liouville equation for a particle under the Lorentz force $Q(E+v\times B)$.[26-28] Quantum corrections appear as powers of $\hbar^2$.

If the electric field depends on the position at most linearly and the magnetic field is homogeneous, the classical Liouville equation is again retrieved.[27,28] This implies that in the dipole approximation for radiation fields [$E(r,t)$ independent of the position $r$, and $B\equiv 0$] all quantum features of the dynamics get lost. Examples of identical results for a classical and a quantum particle under such conditions can readily be picked up in the most recent literature.[34-36]

To appreciate the qualitative nature of the quantum corrections we study the particle in a monochromatic traveling plane wave

$$E(r,t)=\frac{E_0}{2}\exp[-i(\Omega t-q\cdot r)]+\text{c.c.}\,, \quad (5.3)$$

and only look at the electric field term in (5.1). Using the familiar result

$$\exp\left[u\cdot\frac{\partial}{\partial r}\right]f(r)=f(r+u) \quad (5.4)$$

we obtain

$$\frac{Q}{M}\frac{\partial}{\partial v}\cdot\tilde{E}W=\frac{QE_0}{2M}\cdot\frac{\partial}{\partial v}\left[\exp[-i(\Omega t-q\cdot r)]\times\int_{-1/2}^{1/2}d\tau\,W(r,v+\tau v_r,t)\right]+\text{c.c.} \quad (5.5)$$

Here $v_r=\hbar q/M$ is the recoil velocity that the particle would acquire if it could absorb a photon. We ascribe the quantum corrections in (5.1) and (5.2) to the quantized exchange of momentum between the particle and the radiation field, i.e., to recoil effects. In the present theory, and in most approaches to light pressure[10-12] on atoms as well, recoil effects and even the "photon momentum" emerge from the assumption that the position label $r$ of the EM field is replaced with the quantized position of the particle $\hat{r}$. No field commutators, i.e., no photons, need be introduced.

The GIWF theory with fully classical fields neither incorporates "spontaneous" photons emitted by an accelerated charge, nor the associated radiation reaction. Hence the approach is best suited to handle situations which depend on (a large number of) induced absorption and emission processes. For instance, a treatment of the ponderomotive force with quantum corrections could be set up, cf. Ref. 37. However, we neither dwell on the applications of the formulation with purely classical fields any longer, nor do we try to patch up the case of classical fields to include the classical radiation reaction.

## VI. CONCLUDING REMARKS

In this paper we have defined a gauge-invariant Wigner operator and a gauge-independent Wigner function that also incorporate the quantized degrees of freedom of the electromagnetic field, and derived the exact nonrelativistic Heisenberg equation of motion for the GIWO.

The emphasis has been on the case when the field is entirely classical. Then it is possible to define a Weyl transform of operators with all properties familiar from the standard gauge-dependent Weyl transforms. Using the gauge-independent Weyl transforms a quantum-mechanical description of a full experimental run can be provided where the gauge never has to be specified. We have also stressed that in the dipole approximation classical and quantum dynamics are indistinguishable, and qualitatively associated the corrections to the dipole approximation to recoil effects.

The gauge-independent Wigner function automatically avoids all gauge ambiguities, and is particularly well suited to $\hbar$ expansions around the classical counterpart of the quantum problem. Such characteristics may find good use, say, in curing the reliance on an explicitly specified gauge in some free-electron laser theories.[38] However, this is not the path we are going to follow. Since we have worked in the Heisenberg picture and at all stages retained the option of letting the field be quantized, our formulation possesses enough raw power to tackle the quantized radiation reaction. This is the clue to the second paper in this series.[20]

## APPENDIX

### 1. On another Wigner function with vector potential

Occasionally[39–41] a WF that also incorporates the vector potential is introduced simply by treating the ordinary WF (1.9) like a distribution function and changing the variables from $r,p$ to $r,k=p-QA(r)$. As the Jacobian of the transformation is unity, the result is

$$w(r,k)=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}u\cdot[k+QA(r)]\right]\times\langle r-\tfrac{1}{2}u\,|\hat{\rho}|\,r+\tfrac{1}{2}u\rangle\ . \tag{A1}$$

This differs from the definition we have adopted, (1.12), in that the integral over the vector potential is shrunk to one point:

$$\int_{-1/2}^{1/2}d\tau\,A(r+\tau u)\rightarrow A(r)\ .$$

Such a replacement is an identity if $A(r)$ is a linear function of position, but otherwise $w(r,k)$ in (A1) need not coincide with $W(r,k)$ in (1.12).[42]

Under a gauge transformation generated by $\chi(r)$, $w(r,k)$ transforms as follows;

$$\begin{aligned}w'(r,k)&=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}u\cdot[k+QA'(r)]\right]\langle r-\tfrac{1}{2}u\,|\hat{\rho}'|\,r+\tfrac{1}{2}u\rangle\\&=\frac{1}{(2\pi\hbar)^3}\int d^3u\,\exp\left[\frac{i}{\hbar}Q\left[u\cdot\frac{\partial}{\partial r}\chi(r)+\chi(r-\tfrac{1}{2}u)-\chi(r+\tfrac{1}{2}u)\right]\right]\exp\left[\frac{i}{\hbar}u\cdot[k+QA(r)]\right]\langle r-\tfrac{1}{2}u\,|\hat{\rho}|\,r+\tfrac{1}{2}u\rangle\ .\end{aligned} \tag{A2}$$

Unless the generator of the transformation is a linear function of position, in general $w'\neq w$. The WF $w(r,k)$ is gauge dependent.[26,42]

We next consider the use of $w(r,k)$ to calculate expectation values. Changing back to the variables $r,p$ we obtain

$$\int d^3r\,d^3k\,O(r,k)w(r,k)=\int d^3r\,d^3p\,O(r,p-QA(r))W(r,p)\ , \tag{A3}$$

where $W(r,p)$ is the ordinary WF from (1.9). The integral on the left-hand side of (A3) is thus the expectation value of the operator obtained by replacing in $o(r,p)=O(r,p-QA(r))$ the arguments $r,p$ by the operators $\hat{r},\hat{p}$ and symmetrizing with respect to these *canonical* variables. There are trivial exceptions like the pair $O(r,k)=k\leftrightarrow\hat{k}$, but in general no simple ordering rule for $\hat{r}$ and $\hat{k}$ relates the function $O(r,k)$ to the operator $\hat{O}$ whose expectation value is given by (A3).

Finally, if an equation of motion is derived for $w(r,k)$, it usually explicitly contains the electromagnetic potentials. This is easily seen from (4.32c): in the equation of motion for $w(r,k)$ the integral over $\tau$ is obviously absent and $\partial A_C/\partial t$ should be taken at the point $\tau=0$. Hence the higher $\partial/\partial r$ derivatives of the vector potential do not combine with the derivatives of $\phi$ to give derivatives of the electric field. Again, $\phi$ and $A$ that depend on position only linearly constitute an exception.

From the conceptual point of view the WF $w(r,k)$ is a hybrid that gives up both the gauge independence of the WF (1.12) and the simple Weyl correspondence of the usual WF (1.9). Moreover, the change of the variables $k=p-QA$ is not well defined if quantized fields are present, and the quantized radiation reaction cannot easily be incorporated into $w(r,k)$. Nevertheless, thanks to the exceptions listed above, when the fields are all classical and a homogeneous magnetic field or the dipole approximation for radiation is assumed, the shortcomings of $w(r,k)$ need not show up if the potentials are chosen to be linear functions of position. This is typically the case in Refs. 39–41.

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[21]In this paper the caret always denotes an operator. No special notation is used to indicate three-dimensional vectors like $\hat{r},\hat{p},r,p$, etc. However, the Cartesian components 1,2,3 are sometimes given as subscripts to denote components of a vector.

[22]A function of operators is interpreted as formal power series with some prescribed ordering of the operators, or when the function is too singular to be represented as a power series, as a Fourier transform over a set of parameters of a collection of such functions. No attention is paid to convergence problems.

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