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COMMENT

Comment on K-H Yang's energy operator and gauge independent transition amplitudes

T E Feuchtwang, E Kazes and P H Cutler

Physics Department, The Pennsylvania State University, University Park, PA 16802, USA

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Abstract. The purpose of this comment is to discuss critically the energy operator introduced by Yang and collaborators. We also present a critique of the gauge independent transition amplitudes defined by these authors which, we believe, obscures the physical interpretation of transition amplitudes.

In a series of recent publications Yang and collaborators (Yang 1982a, b, 1983a, b, Kobe and Wen 1982) reiterate their observation that the interaction of a material system with the electro-magnetic field involves an energy transfer whose rate is the primary observable quantity; they have interpreted this quantity in terms of Poynting's theorem and showed that

$$\mathrm{d}\mathscr{H}_\mathrm{B}/\mathrm{d}t=\partial\mathscr{H}_\mathrm{B}/\partial t-(\mathrm{i}/\hbar)[\mathscr{H}_\mathrm{B},\mathscr{H}]=\tfrac{1}{2}(\boldsymbol{j}\cdot\boldsymbol{E}+\boldsymbol{E}\cdot\boldsymbol{j}) \tag{1}$$

where the 'energy operator' $\mathscr{H}_\mathrm{B}$ is the 'mechanical' component of the Hamiltonian,

$$\mathscr{H}=(2m)^{-1}[\boldsymbol{p}-(e/c)\boldsymbol{A}]^2+V+eA_0, \tag{2}$$

i.e.

$$\mathscr{H}_\mathrm{B}=\mathscr{H}-eA_0=\tfrac{1}{2}mv^2+V. \tag{3}$$

We note that (1) may also be interpreted in terms of the work–energy theorem.

In this comment we discuss the energy operator and its time dependent spectrum to show that Yang *et al*'s claim that the 'eigenfunctions' of the energy operator are *uniquely* suited for the definition of gauge independent transition amplitudes is incorrect. In fact, we demonstrate that while these transition amplitudes are indeed gauge independent, they are, in general, neither measurable nor do they relate to probabilities of physically significant observations in the study of electromagnetic interactions with matter. Specifically we shall show the following:

(1) There is no *a priori* reason to prefer, as a basis for the expansion of solutions of the Schrödinger equation, the time dependent 'eigenfunctions' $\{\phi_{\varepsilon_j(t)}(t)\}$ belonging to the generally time dependent eigenvalues $\{\varepsilon_j(t)\}$ of the 'energy operator' $\mathscr{H}_\mathrm{B}$.

(2) Yang *et al*'s 'transition amplitudes', while gauge independent, do not generally represent probability amplitudes for an event of either physical interest or simple operational interpretation.

In their analysis, Yang *et al* do not seem to distinguish between gauge covariance of operators, and the gauge independence of their expectation values. The latter follows only if the gauge transform of the operator is equal to its unitary transform $U_\lambda \hat{O} U_\lambda^{-1}$, with $U_\lambda = \exp[\mathrm{i}e\Lambda(\boldsymbol{r}, t)/\hbar c]$ (Feuchtwang *et al* 1984). Noting that $\mathscr{H}_\mathrm{B}$, in contrast to $\mathscr{H}$, satisfies this condition, Yang invokes (1)–(3) to endow $\mathscr{H}_\mathrm{B}$ with a unique physical significance. In particular, they assert that the 'eigenvalue problem' for the time dependent energy operator,

$$[\mathscr{H}_\mathrm{B}(t) - \varepsilon_j(t)]\phi_{\varepsilon_j(t)}(t) = 0, \tag{4}$$

whose eigenvalue spectrum must in general be time dependent, specifies the uniquely preferred and physically significant transition amplitudes

$$a_{\varepsilon_j(t)}(t) = \langle \phi_{\varepsilon_j(t)}(t) | \psi(t) \rangle. \tag{5}$$

There are several serious flaws in this argument, which we shall discuss.

To begin with, we observe that one can always determine a gauge transformation,

$$\boldsymbol{A} \to \boldsymbol{A}' = \boldsymbol{A} + \boldsymbol{\nabla}\Lambda, \qquad A_0 \to A_0' = A_0 - c^{-1}\,\partial\Lambda/\partial t, \tag{6}$$

such that $A_0' = 0$. In such a gauge, $\mathscr{H}'$, the gauge transform of $\mathscr{H}$, and $\mathscr{H}_\mathrm{B}'$, the gauge transform of $\mathscr{H}_\mathrm{B}$, are identical. That is,

$$\mathscr{H}_\mathrm{B}(\boldsymbol{A}') = \mathscr{H}_\mathrm{B}'(\boldsymbol{A}) = \mathscr{H}'(\boldsymbol{A}, A_0) = \mathscr{H}(\boldsymbol{A}'). \tag{7}$$

Here we note parenthetically that, in general, $\mathscr{H}'$ is not a unitary transform of $\mathscr{H}$.

In the following we therefore restrict ourselves, without loss of generality, to the *class of gauges* for which

$$\mathscr{H}_\mathrm{B} = \mathscr{H}. \tag{8}$$

In these gauges Yang's transition amplitudes are the projection of any given solution $\psi(\boldsymbol{r}, t)$, of the Schrödinger equation in the presence of the electromagnetic field,

$$[\mathscr{H} - \mathrm{i}\hbar\,\partial/\partial t]\psi = 0,$$

on the eigenfunctions of the Hamiltonian $\mathscr{H}$, of the same system. However, these are not probability amplitudes of interest in the study of electromagnetic interactions with matter. Rather, what are of interest are the probability amplitudes $a_{\varepsilon_j}(t)$ for finding the system in states of an appropriate *field-free Hamiltonian.*

It is evident that the set $\{\phi_{\varepsilon_j(t)}(t)\}$ defined by

$$[\mathscr{H}(t) - \varepsilon_j(t)]\phi_{\varepsilon_j(t)}(t) = 0 \tag{9}$$

forms a complete basis which can be used in a series expansion of an arbitrary solution, $\psi(\boldsymbol{r}, t)$,

$$|\psi(t)\rangle = \sum_j \langle \phi_{\varepsilon_j(t)}(t) | \psi(t) \rangle | \phi_{\varepsilon_j(t)}(t) \rangle, \tag{10}$$

of the Schrödinger equation.

The 'transition amplitudes'

$$\langle \phi_{\varepsilon_j(t)}(t) | \psi(t) \rangle = a_{\varepsilon_j(t)}(t) \tag{11}$$

are certainly gauge independent, but this is only a necessary and not a sufficient condition for expansion coefficients to represent physically meaningful probability amplitudes. Namely, they have also to correspond to probabilities of events of physical interest and they have to be measurable. We shall now demonstrate that Yang *et al*'s amplitudes do not satisfy either of the latter two conditions.

Yang *et al* do not specify the initial values for the Hamiltonian in (9); we may, however, choose it to be the field-free operator. While this choice appears to establish a connection between $a_{\varepsilon_j(t)}(t)$ and the conventional amplitude $a_{\varepsilon_j}(t)$, nevertheless, the amplitude $a_{\varepsilon_j(t)}(t)$ is still not related in any simple fashion to the (conditional) probability amplitude of finding the system in a field-free state of energy ε_j given that at time $t=0$ it was in a field-free state of energy ε_i. But this is precisely what one wishes to determine in experiments involving the interaction of electromagnetic radiation with matter. Operationally, this probability is determined by counting photons of energy

$$\hbar\omega = \varepsilon_i - \varepsilon_j, \tag{12a}$$

emitted as a result of this 'transition'. On the other hand, if one were to agree with Yang that one really wanted to determine the conditional probability for the system at time t to be in a state of energy $\varepsilon_j(t)$, given that at $t=0$ it was in the field-free state of energy ε_i, then the uncertainty relation $\Delta\varepsilon\,\Delta t > h$ would limit the operational significance of this statement because it would require an instantaneous measurement of the photon energy $\hbar\omega(t)$. That is, while a multichannel analyser can be used to determine the average (i.e. expectation value of the) dissipation of the system, it cannot determine the instantaneous energy of photons which have a continuously variable energy,

$$\hbar\omega(t) = \varepsilon_i - \varepsilon_j(t). \tag{12b}$$

We note that the preceding discussion of the conceptual difficulties associated with the interpretation of the expansion coefficients $a_{\varepsilon_j(t)}(t)$ as transition amplitudes does not apply in its entirety to the electric dipole approximation. In this approximation the energy operator is a unitary transform of the field-free Hamiltonian, $\mathscr{H}_0$,

$$\mathscr{H}_{\rm B} = (2m)^{-1}[\boldsymbol{p} - (e/c)\boldsymbol{A}]^2 + V = U_A(p^2/2m + V)U_A^{-1}, \tag{13}$$

where

$$U_A = \exp[\mathrm{i}e\boldsymbol{A}(t)\cdot(\boldsymbol{r}/\hbar c)]. \tag{14}$$

In the electric dipole approximation $\mathscr{H}_{\rm B}$ and $\mathscr{H}$ are identical, and their eigenvalue spectrum is the same as that of $\mathscr{H}_0$. Furthermore the eigenfunctions $\{\phi_{\varepsilon_j}(t)\}$ of $\mathscr{H}$ and $\{\phi_{\varepsilon_j}\}$ of $\mathscr{H}_0$ are related by the unitary transformation U_A,

$$\phi_{\varepsilon_j}(t) = U_A\phi_{\varepsilon_j}; \tag{15}$$

therefore Yang *et al*'s transition amplitudes satisfy the identity

$$a_j(t) = \langle\phi_{\varepsilon_j}(t)|\psi(t)\rangle = \langle\phi_{\varepsilon_j}|U_A^{-1}\psi(t)\rangle. \tag{16}$$

But $U_A^{-1}\psi(t)$ is a solution of the Schrödinger equation,

$$(\{U_A^{-1}\mathscr{H}U_A - U_A^{-1}[\mathrm{i}\hbar(\partial/\partial t)U_A]\} - \mathrm{i}\hbar(\partial/\partial t))U_A^{-1}\psi = 0. \tag{17}$$

That is, the time evolution of $U_A^{-1}\psi$ is governed by the Hamiltonian

$$\mathscr{H}' = \mathscr{H}_0 - (e/c)(\partial\boldsymbol{A}/\partial t)\cdot\boldsymbol{r}. \tag{18}$$

Thus in this simple case, Yang *et al*'s definition of transition amplitudes is equivalent to the conventional definition in a particular gauge. The solution of the Schrödinger equation with $\mathscr{H}'$ as the Hamiltonian is projected on the eigenfunctions of the field-free Hamiltonian, $\mathscr{H}_0$. It is important to recognise that by defining the conventional transition amplitudes in terms of $\mathscr{H}'$ one explicitly singles out an 'initial' or preferred gauge.

Finally we note that due to the well known non-uniqueness of the classical mechanical Lagrangian previously discussed by us (Feuchtwang *et al* 1983a, b, Kazes *et al* 1983), there exists a large class of 'energy operators', $\mathscr{H}_B[f]$, all of which satisfy the *gauge independent formulation* of (1), namely that the expectation value of the total time derivative of $\mathscr{H}_B[f]$ is the mean dissipation:

$$\langle\psi[f]|\mathrm{d}\mathscr{H}_B[f]/\mathrm{d}t|\psi[f]\rangle = \tfrac{1}{2}\langle \boldsymbol{j}\cdot\boldsymbol{E}+\boldsymbol{E}\cdot\boldsymbol{j}\rangle \tag{19}$$

where

$$(\mathrm{i}\hbar(\partial/\partial t)-\mathscr{H}[f])\psi[f]=0, \tag{20}$$

$$\mathscr{H}[f]=(2m)^{-1}[\boldsymbol{p}-(e/c)\boldsymbol{A}+\boldsymbol{\nabla}f]^2+V+eA_0+\partial f/\partial t. \tag{21}$$

The function f arises from the total time derivative $\mathrm{d}f/\mathrm{d}t$ which can be added to the classical Lagrangian without affecting the equations of motion. We shall impose on f the condition

$$eA_0=-\partial f/\partial t, \tag{22}$$

so that $\mathscr{H}[f]$ reduces to an 'energy operator', in the sense of (2) and (3). We emphasise that the right-hand side of (19) is independent of f.

It is evident that the projections of $\psi(t)$ on the set of eigenfunctions, $\{\phi_{\varepsilon_j}([f])\}$, of any one of the class of energy operators $\mathscr{H}_B[f]$ are explicitly gauge invariant quantities, and, following Yang *et al*'s argument, could have been chosen to define a set of gauge invariant transition amplitudes,

$$a_{\varepsilon_j(t)}[f]=\langle\phi_{\varepsilon_j(t)}[f]|\psi(t)\rangle. \tag{23}$$

This illustrates once more the general non-uniqueness of transition amplitudes in the presence of electromagnetic fields, which, as we noted above, is traceable to the corresponding non-uniqueness of the Lagrangian formulation of classical mechanics.

In conclusion, we have shown the following.

(1) The energy operator introduced by Yang is one of a large class of operators all of which satisfy (1)–(3). Thus, there is nothing unique about Yang's particular choice.

(2) There is no *a priori* reason to prefer the time dependent 'eigenfunctions' $\{\phi_{\varepsilon_j(t)}(t)\}$ of any of the 'energy operators' $\mathscr{H}_B$ as a basis for the expansion of solutions of the Schrödinger equation, since, in general, they involve time dependent energy eigenvalues which cannot be measured precisely.

(3) In the presence of fields, Yang *et al*'s transition amplitudes still exhibit the non-uniqueness traceable to the corresponding non-uniqueness of the Lagrangian formulation of classical mechanics†. The gauge independent formulations of quantum

† The determination of gauge independent transition amplitudes at any time after the external fields have been switched off, discussed by Feuchtwang *et al* (1983b), is not affected by this non-uniqueness of the Lagrangian.

mechanics exhibit a corresponding non-uniqueness (Feuchtwang *et al* 1983a, b, Kazes *et al* 1983, DeWitt 1962, Mandelstam 1962, Belinfante 1962, Aharonov and Bohm 1962).

(4) The energy operator and its eigenfunctions provide Yang *et al* with a basis set exhibiting an explicit gauge dependence, which cancels the bothersome gauge dependence of the expansion coefficients, or 'transition amplitudes'. In this sense Yang *et al*'s approach is similar to that discussed by Feuchtwang *et al* (1983a). However, in contrast to the latter approach, the procedure advocated by Yang and collaborators leads, in general, to 'transition amplitudes' which, while they are gauge independent, generally do not represent probability amplitudes for an event of either physical interest or simple operational interpretation.

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References

Aharonov Y and Bohm D 1962 *Phys. Rev.* **125** 2192
Belifante F J 1962 *Phys. Rev.* **128** 2832
DeWitt B S 1962 *Phys. Rev.* **125** 2189
Feuchtwang T E, Kazes E, Grotch H and Cutler P H 1983a *Phys. Lett.* A **93** 4
—— 1984 *J. Phys. A: Math. Gen.* **17** 151
Kazes E, Feuchtwang T E, Grotch H and Cutler P H 1983 *Phys. Rev.* D **21** 1388
Kobe D H and Wen E C-T 1982 *J. Phys. A: Math. Gen.* **15** 787
Mandelstam S 1962 *Ann. Phys.* **19** 1
Yang K-H 1982a *J. Phys. A: Math. Gen.* **15** 437
—— 1982b *J. Phys. A: Math Gen.* **15** 1201
—— 1983a *J. Phys. A: Math. Gen.* **16** 919
—— 1983b *J. Phys. A: Math. Gen.* **16** 935