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A NOTE ON GAUGE INVARIANCE IN PERTURBATION THEORY

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This paper discusses gauge invariance issues in semiclassical perturbation theory, outlining a nonrelativistic single-particle treatment which guarantees perturbative gauge invariance in a relative sense (that is, in relationship to a chosen "reference" gauge of the electromagnetic four-potential). The selection of the reference gauge depends on the intended physical meanings of the calculated quantities, but it appears that the transverse gauge is the most appropriate choice. Generalizations to multiparticle systems and relativistic particles are possible.

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1. Introduction

A classical, single-particle nonrelativistic Hamiltonian formalism is introduced (Sect. 2, Appendix A), similar to the one employed for reparametrization invariant Lagrangian systems [1, 2]. This allows a (four-dimensional) treatment of time and space on equal footing, a convenient feature for the use of the minimal replacement in the presence of an external electromagnetic (EM) perturbation (Sect. 4). The unperturbed quantum states are examined in Sect. 3, pointing out that the canonical momentum operators possess a gauge freedom (Sect. 2). At the quantum level, the minimal replacement is done in a fixed gauge for the EM interaction (Sect. 4), but the gauge freedom of the momentum operators produces exact equations which are fully invariant with respect to gauge changes of the four-potential (Sect. 5). In perturbation theory, the invariance is only relative, with the originally chosen EM gauge acting as a reference (Sect. 5, Appendix B). The selection of this reference relates to the intended meanings of the calculated quantities, but it appears that the transverse gauge is the most appropriate choice (Sect. 6). For a discussion of a variety of issues relating to gauge choices, see also Ref. [3].

Notation is rather conventional. Specifically, Greek indices run through the values $0, 1, 2, 3$ and the Latin index ℓ takes on the values $1, 2, 3$; other labels are defined as needed. The summation convention is applied to repeated up and down indices, and units are such that $\hbar = c = 1$. An attempt is made at distinguishing powers from superscripts: for instance, $(m)^2$ is a power, while x^2 indicates a specific variable with superscript 2. The curly bracket notation is used for ordered sets: e.g., $\{x^\lambda\}$ denotes four objects in the order $0 - 3$.

2. Momentum operators

In a given frame[1] of reference $\mathcal{X}$ of real space-time coordinates $x = \{x^\lambda\} = \{t, x^\ell\}$ and pseudoeuclidean metric $g_{\mu\nu} = g^{\mu\nu} = \mathrm{diag}(+1, -1, -1, -1)$, consider a particle of rest mass $m > 0$ described classically by its space-time position $x(\tau)$, where $\tau \in \Re$ is an evolution parameter [2, 4]. For a nonrelativistic treatment, introduce the mechanical momentum $\pi = \{\pi_\lambda\}$, letting $\pi^\ell = -\pi_\ell$ be the vector components

$$\pi^\ell = m \frac{\mathrm{d}x^\ell}{\mathrm{d}t}\,, \tag{1}$$

and $\pi^0 = \pi_0$ indicate the particle's energy

$$\pi^0 = V(x) + \frac{m}{2} \sum_{\ell=1}^{3} \left(\frac{\mathrm{d}x^\ell}{\mathrm{d}t} \right)^2 . \tag{2}$$

As customary, the components π_ℓ are purely kinetic, whereas π_0 adds the kinetic energy to a (real) potential $V(x)$, measured in reference to a chosen "ground" $\overline{x}$ such that $V(\overline{x}) = 0$.

For now, consider Hamiltonian formulations such that the canonical momentum $p = \{p_\lambda\}$ is the same as the mechanical momentum π. For example, choosing $\tau = t$ as the evolution parameter, take the "extended" Hamiltonian [2, 4]

$$K(x, p) = p_0 - V(x) - \frac{1}{2m} \left[(p_1)^2 + (p_2)^2 + (p_3)^2 \right], \tag{3}$$

coupled to the constraint

$$K(x, p) = 0\,. \tag{4}$$

(See Appendix A for more details.)

Then, the quantum mechanical description can be started from the commutation rules

$$[\mathcal{P}_\mu\,, x^\nu] = \mathrm{i}\, \delta_\mu^{\ \nu}\,, \tag{5}$$

[1] Changes of coordinates will not be examined in detail.

and

$$[\mathcal{P}_\mu , \mathcal{P}_\nu] = \mathcal{O} \,, \tag{6}$$

where $\mathcal{O}$ is the null operator. Here, $\mathcal{P} = \{\mathcal{P}_\lambda\}$ are the linear hermitian operators corresponding to p in the coordinate representation, and are given by [5, 6]:

$$\mathcal{P}_\mu = \Delta_\mu(x) + \mathrm{i}\,\partial_\mu \,, \tag{7}$$

with

$$\Delta_\mu(x) = \partial_\mu \Delta(x) \,, \tag{8}$$

where $\Delta(x)$ is a well-behaved, arbitrary real function. The special "gauge"

$$\mathcal{P}^\sharp_\mu = \mathrm{i}\,\partial_\mu \tag{9}$$

is often chosen in the literature [5, 6]. The coincidence of p and π makes the quantization procedure reasonably transparent and unambiguous; specifically, it is clear that the gauge freedom of $\mathcal{P}$ originates from the commutators, not from ambiguities in the classical p's, as these have the physical meanings specified by π. In later sections, p and π will no longer coincide; the fundamental quantization rule will remain as: $p \to \mathcal{P}$, where $\mathcal{P}$ satisfies Eqs. (5)–(8).

Remark. For definiteness, the description based on Eqs. (3) and (4) will be the only one examined in the following; relativistic particles, multiparticle systems, or systems without a clear classical analog will not be considered here explicitely (however, these generalizations are possible).

It is noted that the variable t plays a double role in the outlined treatment: as a coordinate, and as the evolution parameter. This creates a possible conflict, because the consistency of the quantization procedure $p \to \mathcal{P}$ presumes that $\mathrm{d}\tau$ is left unchanged[2] by passive transformations of coordinates $x \to x'$. Luckily, $\mathrm{d}t$ is nearly an invariant in nonrelativistic physics, and is only changed by the inversion: $t' = -t +$ const. Hence, either this inversion is disallowed, or needs to be accommodated by means of a slight modification of the classical formalism, e.g., by redefining $\tau = t$ (if t runs forward in relationship to the macroscopic arrow of time) and $\tau = -t$ (otherwise); then, $\pi^\ell = m\,\mathrm{d}x^\ell/\mathrm{d}\tau$, and so on. In this paper, the forward t option is assumed, with no inversion.

3. *Unperturbed states*

Before the EM interaction is introduced, the unperturbed wave functions are chosen by means of compatible eigenvalue equations of the type

$$L_{(n)}(x, \mathcal{P})\, \Phi_\varepsilon(x) = \varepsilon_{(n)} \Phi_\varepsilon(x) \,, \tag{10}$$

[2]Changes of the evolution parameter (not detailed in this paper) go under the name of reparametrizations, and are independent of the coordinate transformations [1, 2].

where $\varepsilon = \{\varepsilon_{(n)}\}$ are the eigenvalues and $n = 0, 1, \dots$ numbers the equations needed to specify the states completely (up to normalization). In the special gauge $\mathcal{P}^\sharp$, Eq. (10) is written as

$$L_{(n)}(x, \mathcal{P}^\sharp)\, \Phi^\sharp_\varepsilon(x) = \varepsilon_{(n)} \Phi^\sharp_\varepsilon(x)\,, \tag{11}$$

and the normalized eigenfunctions are related by

$$\Phi_\varepsilon(x) = \exp\{\mathrm{i}[\Delta(x) + C_\varepsilon]\}\; \Phi^\sharp_\varepsilon(x)\,, \tag{12}$$

where C_ε is a real constant (which can be chosen to vanish with no loss of generality). The linear hermitian operators $L_{(n)}$ in Eqs. (10) and (11) originate from appropriate conserved classical quantities $L_{(n)}(x,p)$, under the replacement of p with $\mathcal{P}$ or $\mathcal{P}^\sharp$. For example, if the classical conserved function $L_{(1)}(x,p)$ is $L_{(1)} = p_0$, the corresponding quantum eigenvalue $\varepsilon_{(1)}$ represents the observed particle's energy. The Schrödinger equation is included ($n = 0$), written as an eigenvalue problem with a vanishing eigenvalue $\varepsilon_{(0)} = 0$; the function $L_{(0)}$ coincides with the Hamiltonian K.

4. *Electromagnetic interaction*

In the presence of the interaction with an EM field of components $F_{\mu\nu}$ and (real) four-potential $A = \{A_\lambda\}$ such that

$$F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)\,, \tag{13}$$

the unperturbed Hamiltonian function K is usually modified [7] as follows (minimal replacement),

$$p_\mu \to p_\mu - qA_\mu(x)\,, \tag{14}$$

where $q \in \Re - \{0\}$ is the particle's electric charge. This amounts to a difference between p and π given by

$$p_\mu = \pi_\mu + qA_\mu(x)\,, \tag{15}$$

with π formally defined as in Sect. 2. The canonical momentum p (although not invariant under gauge changes of A) may be interpreted as the particle's total momentum, resulting from mechanical and EM contributions [7]. Specifically, any definite choice of the gauge of A implies a convention on how much EM momentum belongs to particles, versus how much is attributed to the field (see also Sect. 6).

For a given $F_{\mu\nu}$, the corresponding four-potential A is arbitrary by a gauge transformation [7, 8]. A special gauge (transverse gauge) may be selected, which makes the four-potential physically significant and unique [9]; the symbol $A^\sharp$ will indicate this choice. All other choices are obtained by means of the gauge freedom

$$A_\mu(x) = A^\sharp_\mu(x) + \partial_\mu\Gamma(x)\,, \tag{16}$$

where $\Gamma(x)$ is any well-behaved real function.

For quantization, it is convenient (and correct) to use the $A^\sharp$ replacements

$$\mathcal{P}_\mu \to \mathcal{P}_\mu - qA^\sharp_\mu(x)\,, \tag{17}$$

or

$$\mathcal{P}^\sharp_\mu \to \mathcal{P}^\sharp_\mu - qA^\sharp_\mu(x)\,, \tag{18}$$

which have a long tradition in the literature [9]. The next section will discuss this type of replacements in relationship to gauge freedom.

5. *Perturbation theory*

In presence of the interaction (13), the replacement (17) transforms the unperturbed Hamiltonian operator $K(x, \mathcal{P})$ into $K(x, \mathcal{P} - qA^\sharp)$, where

$$\mathcal{P}_\mu - qA^\sharp_\mu(x) = [\Delta_\mu(x) + \mathrm{i}\,\partial_\mu] - qA^\sharp_\mu(x) = \mathrm{i}\,\partial_\mu - qA_\mu(x)\,, \tag{19}$$

with the definition

$$A_\mu(x) = A^\sharp_\mu(x) + \partial_\mu \left[-\frac{\Delta(x)}{q} \right], \tag{20}$$

corresponding to

$$\Delta_\mu(x) = q\,[A^\sharp_\mu(x) - A_\mu(x)]\,. \tag{21}$$

Since the function Δ is arbitrary, the original four-potential $A^\sharp$ may be put into any possible gauge A by means of Eqs. (20) and (21). Thus, the operator

$$K(x, \mathcal{P} - qA^\sharp) = K(x, \mathrm{i}\partial - qA) \tag{22}$$

displays the usual EM quantum gauge invariance [6, 7] in relationship to the equation (Schrödinger equation with EM interaction)

$$K(x, \mathrm{i}\partial - qA)\,\Psi(x) = 0\,. \tag{23}$$

Here, $\Psi(x)$ indicates a wave-function and the notation $\partial = \{\partial_\lambda\}$ has been introduced. In addition to Eq. (23), other compatible gauge-invariant equations of a similar form

$$W(x, \mathrm{i}\partial - qA)\,\Psi(x) = \omega\,\Psi(x)\,, \qquad \omega \in \Re\,, \tag{24}$$

may be possible. In all cases of this type, the special gauge $\mathcal{P}^\sharp$ produces equations written in the transverse gauge of the four-potential. For instance, starting from $K(x, \mathcal{P}^\sharp)$ and using (18), one obtains

$$K(x, \mathrm{i}\partial - qA^\sharp)\,\Psi^\sharp(x) = 0\,, \tag{25}$$

in place of Eq. (23).

Equations like (23)–(25) are called "exact" equations, although they provide only a partial description of the physics associated with EM interactions. A more precise formalism would have to include and quantize the nonhomogeneous EM field [7] equations (with one of the sources being the four-current of the charge q itself). At any rate, even when $F_{\mu\nu}$ is treated as a given classical external field (which is the approach of this paper), the exact equations are typically difficult to solve, and perturbation theory is often introduced.

In rather general terms, all perturbative calculations [7] are characterized by the application of linear hermitian operators of the type

$$\left[R(x, \mathcal{P} - qA^\sharp) + S(x, \mathcal{P})\right] \tag{26}$$

on states like those specified in Sect. 3. Thus, it is interesting to compare the results

$$\Upsilon_\varepsilon(x) = \left[R(x, \mathcal{P} - qA^\sharp) + S(x, \mathcal{P})\right] \Phi_\varepsilon(x)\,, \tag{27}$$

and

$$\Upsilon^\sharp_\varepsilon(x) = \left[R(x, \mathcal{P}^\sharp - qA^\sharp) + S(x, \mathcal{P}^\sharp)\right] \Phi^\sharp_\varepsilon(x)\,. \tag{28}$$

Making use of Eqs. (19)–(21), these expressions can also be written as

$$\Upsilon_\varepsilon(x) = \left[R(x, \mathrm{i}\partial - qA) + S(x, \mathrm{i}\partial + D)\right] \Phi_\varepsilon(x)\,, \tag{29}$$

and

$$\Upsilon^\sharp_\varepsilon(x) = \left[R(x, \mathrm{i}\partial - qA^\sharp) + S(x, \mathrm{i}\partial)\right] \Phi^\sharp_\varepsilon(x)\,, \tag{30}$$

from which, with the help of Eq. (12):

$$\Upsilon_\varepsilon(x) = \exp\left\{\mathrm{i}[\Delta(x) + C_\varepsilon]\right\}\, \Upsilon^\sharp_\varepsilon(x)\,. \tag{31}$$

Here, the notation $D = \{\Delta_\lambda\}$ was introduced at Eq. (29). For a concrete example of a perturbative approach, one may start from the Hamiltonian of Eq. (3) with the unperturbed quantum states (10), in order to obtain the perturbative operator (26) corresponding to the particle's change in total energy [10, 11] due to the EM interaction (interaction energy operator). This can be done by defining

$$R(x, \mathcal{P}) = -K(x, \mathcal{P})\,, \tag{32}$$

and

$$S(x, \mathcal{P}) = [\,\text{other EM interaction terms}\,] - R(x, \mathcal{P})\,. \tag{33}$$

(See also Appendix B.) The expression in square brackets denotes interactive energy terms containing $F_{\mu\nu}$ (but not its four-potential) which cannot be generated from the minimal replacement. For instance, the minimal replacement in a spinless model

Hamiltonian like (3) produces no EM spin interactions: if needed, all spin effects must be inserted "by hand" [10, 11].

From Eqs. (27)–(31), it is deduced that perturbation theory (calculated in terms of suitable matrix elements) is gauge-invariant as described above, but only in a relative sense. That is, each perturbative calculation agrees with the corresponding calculation performed in the transverse gauge of the four-potential; $A^\sharp$ is used as a reference gauge. If this reference is changed into

$$A^{\sharp\sharp}_\mu(x) = A^\sharp_\mu(x) + \partial_\mu \Gamma^{\sharp\sharp}(x) \,, \tag{34}$$

at the level of Eqs. (17) and (18), the new perturbative calculations may not agree with the old. Conceptually, this is not a major flaw, because the exact equations are fully gauge-invariant (hence, independent of the reference). Nevertheless, one must justify why $A^\sharp$ is the appropriate choice for those calculations where the reference gauge does matter. This issue will be addressed in the next section.

6. *Reference gauge*

For a given $F_{\mu\nu}$ vanishing with sufficient rapidity at spatial infinity[3], the four-potential $A^\sharp$ is the only solution A of Eq. (13) with components A_μ vanishing at spatial infinity and satisfying the constraint [7, 9]

$$\partial_\ell A^\ell(x) = 0 \,. \tag{35}$$

To some extent, the choice of $A^\sharp$ as the reference gauge for perturbative calculations is a matter of convention, in that it relates to the intended meanings of the calculated quantities. For example, in the case of Eqs. (32) and (33), the interpretation of (26) as the particle's interaction energy operator depends on having established a convention on how much EM energy and vector momentum pertain to particles, versus how much belong to the field. Specifically, the transverse gauge attributes to the (spinless) particles in the field all of the EM energy (and vector momentum) which are not in the form of EM radiation [7]. This can be shown by examining the classical EM theory in some detail (see part III of chapter XXI of Ref. [7]).

Hence, it appears that the transverse gauge is a more suitable reference than others for performing perturbative calculations comparable to experiment; for instance, the particle's interaction energy is determined by measuring (directly or indirectly) its energy exchanges with a radiation field. This corresponds to the type of "bookkeeping" prescribed by the transverse gauge, which separates the radiation (i.e., transverse) field from the rest of the EM environment.

[3] Highly idealized situations (e.g., a magnetic field which is constant and uniform throughout space-time) can be corrected by the introduction of appropriate "damping" factors, in order to obtain a more realistic behaviour at spatial infinity.

7. *Conclusions*

Generalizations to nonrelativistic multiparticle systems are possible, as well as to relativistic cases (i.e., Dirac equation and Klein-Gordon equation), or nonrelativistic cases with relativistic corrections. The existence of a reference gauge for perturbation theory relates to the intrinsic ambiguity in the distinction of particle attributes from field attributes; this ambiguity is solved *de facto* by the experimental procedures.

Appendix A. Hamiltonian formalism

This is a brief review of the Hamiltonian formalism associated with Eqs. (3) and (4). In general, if a Hamiltonian function $H(x, p)$ is given, the corresponding canonical equations for $x(\tau)$ and $p(\tau)$ are as follows [2]

$$\frac{\mathrm{d}x^\mu}{\mathrm{d}\tau} = \frac{\partial H(x,p)}{\partial p_\mu} , \qquad \frac{\mathrm{d}p_\mu}{\mathrm{d}\tau} = -\frac{\partial H(x,p)}{\partial x^\mu} . \tag{36}$$

Specifically for the Hamiltonian K of Eq. (3), this reads as

$$\frac{\mathrm{d}x^0}{\mathrm{d}t} = 1 , \qquad \frac{\mathrm{d}x^\ell}{\mathrm{d}t} = -\frac{p_\ell}{m} , \tag{37}$$

and

$$\frac{\mathrm{d}p_\mu}{\mathrm{d}t} = \frac{\partial V(x)}{\partial x^\mu} , \tag{38}$$

while the constraint (4) represents the definition

$$p_0 = V(x) + \frac{1}{2m}\left[(p_1)^2 + (p_2)^2 + (p_3)^2\right] . \tag{39}$$

After the EM field $F_{\mu\nu}$ is introduced, modify the unperturbed function K of Eq. (3) into the new function

$$\widetilde{K}(x,p) = K(x, p - qA) , \tag{40}$$

and use $\widetilde{K}$ as the Hamiltonian for Eq. (36); then, take into account the constraint

$$\widetilde{K}(x,p) = 0 . \tag{41}$$

It is readily proved that this type of classical treatment leads to results for $x(t)$ that are invariant under gauge changes of the four-potential. In fact, one obtains

$$\frac{\mathrm{d}x^0}{\mathrm{d}t} = 1 , \qquad \frac{\mathrm{d}x^\ell}{\mathrm{d}t} = -\left[\frac{p_\ell - qA_\ell(x)}{m}\right] , \tag{42}$$

and

$$\frac{\mathrm{d}p_\mu}{\mathrm{d}t} = \frac{\partial\,[V(x) + qA_0(x)]}{\partial x^\mu} + q\left[\frac{p_\ell - qA_\ell(x)}{m}\right]\left[\frac{\partial A^\ell(x)}{\partial x^\mu}\right], \tag{43}$$

which combine as

$$\frac{\mathrm{d}^2 x^\ell}{\mathrm{d}t^2} = -\frac{1}{m}\left[\frac{\partial V(x)}{\partial x^\ell}\right] + \left[\frac{q}{m}\,F^\ell{}_\alpha(x)\right]\left(\frac{\mathrm{d}x^\alpha}{\mathrm{d}t}\right), \tag{44}$$

with the constraint (41) giving the definition

$$p_0 = [V(x) + qA_0(x)] + \frac{1}{2m}\sum_{\ell=1}^{3}\left[p_\ell - qA_\ell(x)\right]^2. \tag{45}$$

The outlined formulation presumes that $F_{\mu\nu}$ is a given external field, strictly vanishing in the case of Eqs. (37)–(39). A more complete (and complex) description would have to include the nonhomogeneous EM field equations, with one of the sources being the charge q itself [7]. This feedback mechanism generates the classical emission of EM radiation by accelerated particles [12]; at the quantum level, the appropriate theory becomes quantum electrodynamics [13].

In closing, note that Eq. (36) generates the usual Poisson bracket structure of classical mechanics [2]

$$\frac{\mathrm{d}Z}{\mathrm{d}\tau} = \frac{\partial Z(x,p)}{\partial x^\alpha}\,\frac{\partial H(x,p)}{\partial p_\alpha} - \frac{\partial Z(x,p)}{\partial p_\alpha}\,\frac{\partial H(x,p)}{\partial x^\alpha}\,. \tag{46}$$

If $\mathrm{d}Z/\mathrm{d}\tau = 0$, the quantity $Z(x,p)$ is conserved.

Appendix B. Interaction

Here are provided some details relating to Sect. 5. Consider the interaction energy operator discussed therein, given by

$$\mathcal{I} = -K(x, \mathrm{i}\partial - qA) + K(x, \mathcal{P}), \tag{47}$$

having disregarded the terms in square bracket at Eq. (33). After some algebra, it may be written as

$$\mathcal{I} = qA_0^\sharp(x) - \frac{(q)^2}{2m}\sum_{\ell=1}^{3}[A_\ell^\sharp(x)]^2 - \frac{\mathrm{i}q}{m}\sum_{\ell=1}^{3}A_\ell^\sharp(x)\left[\partial_\ell + \mathrm{i}qA_\ell(x)\right]. \tag{48}$$

It is reminded that the gauge of A and that of $\mathcal{P}$ at Eq. (47) are linked by Eq. (21). For this reason, and irrespective of the gauge of A, the expression (48) contains the gauge covariant derivatives $\partial_\ell + \mathrm{i}qA_\ell$ and the four-potential reduced to its tranverse reference gauge; such an operator allows for the type of gauge invariance shown at Eqs. (27)–(31).

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BILJEŠKA O BAŽDARNOJ INVARIJANTNOSTI U TEORIJI SMETNJI

U radu se raspravljaju pitanja baždarne invarijantnosti u poluklasičnoj teoriji smetnji, opisujući nerelativistički jednočestični račun koji osigurava baždarnu invarijantnost smetnje (tj., u odnosu prema odabranoj referentnoj baždarnosti elektromagnetskog četiri-potencijala). Odabir referentne baždarnosti ovisi o željenom fizičkom značenju računatih veličina, ali se čini da je poprečna baždarnost najpovoljniji odabir. Moguća su poopćenja na višečestične sustave i relativističke čestice.