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On non-relativistic electron theory

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ABSTRACT. — A discussion of non-relativistic electron theory, which makes use of the electromagnetic field *potentials* only as useful working variables in the intermediate stages, is presented. The separation of the (transverse) radiation field from the longitudinal electric field due to the sources is automatic, and as a result, this formalism is often more convenient than the usual Coulomb gauge theory used in molecular physics.

RÉSUMÉ. — L'article présente la discussion d'une théorie non-relativiste de l'électron qui se sert uniquement des potentiels électromagnétiques dans les étapes intermédiaires du calcul. Comme la séparation entre le champ (transversal) de la radiation et le champ longitudinal dû aux sources est automatique, ce formalisme est mieux adapté à la physique moléculaire que la théorie classique de la jauge de Coulomb.

1. INTRODUCTION

In classical physics the equation of motion for a particle of mass m, charge e, position coordinate $\underline{\mathrm{R}}(t)$, and momentum $\underline{p}(t)$, under the influence of a specified electromagnetic field $\{ \underline{\mathrm{E}}(\underline{x}, t), \underline{\mathrm{B}}(\underline{x}, t) \}$ is given by Newton's second law, $\underline{\mathrm{F}} = d\underline{p}/dt$, with the Lorentz Force $\underline{\mathrm{F}}$,

$$\underline{\mathrm{F}}(\underline{\mathrm{R}}, \dot{\underline{\mathrm{R}}}, t) = e \{ \underline{\mathrm{E}}(\underline{\mathrm{R}}, t) + \dot{\underline{\mathrm{R}}} \wedge \underline{\mathrm{B}}(\underline{\mathrm{R}},) \, t \}. \tag{1}$$

Although the classical theory can provide a guide to the form of the corresponding quantum theory, the Newtonian formalism is not very convenient and it is customary to reformulate the classical dynamical theory in a lagrangian (or hamiltonian) form before passing to the quantum theory. In the lagrangian method we require a quantity L which is such that the Euler-Lagrange equation

$$\left(\frac{\partial L}{\partial \underline{R}}\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{\underline{R}}}\right) \equiv \underline{\mathscr{L}}[L] = 0 \tag{2}$$

is equivalent to equation (1). In the evaluation of equation (2), which serves to define the operator $\underline{\mathscr{L}}$, it is assumed that the fields are given functions of the particle variables. If one wishes to study the behaviour of the field as well, one has to add to L a lagrangian for the field, and then show that the combination of the two parts leads to the Maxwell equations when the fields are varied and the particle variables are held constant.

Although the usual discussion of this problem employs certain auxiliary quantities (the field potentials) instead of the physically important field strengths, it is also possible to develop a hamiltonian scheme of non-relativistic electrodynamics which uses the canonical particle variables $\{ \underline{R}, \underline{p} \}$ and the electric and magnetic field variables $\{ \underline{E}(\underline{x}, t), \underline{B}(\underline{x}, t) \}$. This result is achieved at the expense of the introduction of certain (arbitrary) spatial curves which occur in path integrals involving the electromagnetic field variables. The field potentials are used simply as convenient working variables in the intermediate steps. A special case of this alternative formalism was discussed by Atkins and Woolley who showed how one could develop a hamiltonian description of the interaction of neutral molecular systems with radiation in terms of the molecular multipole moments and the electromagnetic field variables [*1*]. Less general formulations of the same kind have also been given recently by Hansen [*2*] and by Stenholm and Savolainen [*3*], [*4*]. The molecular multipoles are introduced via the microscopic electric and magnetic polarization fields, $\underline{P}(\underline{x}, t)$ and $\underline{M}(\underline{x}, t)$ respectively, which replace the usual charge and current densities in the interaction energies. These polarization fields have previously been used extensively in discussions of the statistical mechanics of the Maxwell equations [*5*]-[*7*].

In this paper we shall show that the polarization field formalism may still be achieved even when the use of a multipole expansion is not appropriate and thereby place it on a better foundation; to emphasize this point we shall confine our attention initially to the electrodynamics of a single charged particle. The multipolar representation which is useful in molecular physics may be recovered if required by making a Taylor series expansion of the path integrals referred to above. It should be noted that although the field potentials are dispensed with, there is no difficulty in describing the interference phenomenon discussed by Bohm and Aharonov [*8*], [*9*]; this is because the use of path integrals introduces into the theory precisely the kind of non-locality that is required to describe their effect.

2. THE LAGRANGIAN AND THE EULER-LAGRANGE EQUATIONS

We propose to study in this section a lagrangian for a non-relativistic charged particle interacting with the electromagnetic field which may be written in the form (in S. I. units)

$$L = \frac{1}{2} m\dot{\underline{R}}^2 + \int d^3x \underline{P}(\underline{x}, t).\underline{E}(\underline{x}, t) + \int d^3x \underline{M}(\underline{x}, t).\underline{B}(\underline{x}, t) - \frac{1}{2}\varepsilon_0 \int d^3\underline{x} \{ \underline{E}(\underline{x}, t).\underline{E}(\underline{x}, t) - c^2 \underline{B}(\underline{x}, t).\underline{B}(\underline{x}, t) \} \quad (3)$$

where the particle-field coupling terms are expressed in terms of the electromagnetic field variables, and the electric and magnetic polarization fields, $\underline{P}(\underline{x}, t)$ and $\underline{M}(\underline{x}, t)$ respectively. These polarization densities are related to the usual charge and current densities by the equations,

$$\begin{aligned} \rho(\underline{x}, t) &\equiv e\delta(\underline{R} - \underline{x}) = - \underline{\nabla}.\underline{P}(\underline{x}, t) \\ \underline{j}(\underline{x}, t) &\equiv e\dot{\underline{R}}\delta(\underline{R} - \underline{x}) = \frac{d\underline{P}(\underline{x}, t)}{dt} + \underline{\nabla} \wedge \underline{M}(\underline{x}, t) \end{aligned} \quad (4)$$

from which one infers at once that equivalent fields $\underline{P}'(\underline{x}, t)$ and $\underline{M}'(\underline{x}, t)$ defined by,

$$\begin{aligned} \underline{P}'(\underline{x}, t) &= \underline{P}(\underline{x}, t) + \underline{\nabla} \wedge \underline{C}(\underline{x}, t) \\ \underline{M}'(\underline{x}, t) &= \underline{M}(\underline{x}, t) - \frac{d\underline{C}(\underline{x}, t)}{dt} \end{aligned} \quad (5)$$

where $\underline{C}(\underline{x}, t)$ is an arbitrary, differentiable vector field, also satisfy equation (4). Thus equation (3) which replaces the usual expression involving the arbitrary potentials, has transferred the arbitrariness to quantities depending on the particle variables $\underline{R}$ and $\dot{\underline{R}}$.

In order to recover the Maxwell equations from (3) using the Principle of Least Action it is necessary to introduce the field potentials $\phi(\underline{x}, t)$ and $\underline{A}(\underline{x}, t)$ as the lagrangian variables (*) through the implicit definitions

$$\begin{aligned} \underline{B}(\underline{x}, t) &= \underline{\nabla} \wedge \underline{A}(\underline{x}, t) \\ \underline{E}(\underline{x}, t) &= - \underline{\nabla}\phi(\underline{x}, t) - \frac{\partial \underline{A}(\underline{x}, t)}{\partial t}. \end{aligned} \quad (6)$$

(*) This is because the Least Action formulation requires that the equations of motion be (at least) second order differential equations in the lagrangian variables; this is true of the Maxwell equations expressed in terms of ϕ and $\underline{A}$ but not when expressed in terms of $\underline{E}$ and $\underline{B}$. Since the starting equations of motion and the final hamiltonian are independent of ϕ and $\underline{A}$ one might expect there to be a method of passing directly from one to the other without introducing ϕ and $\underline{A}$.

It is then a straightforward matter to verify that one obtains the equations of motion in the form,

$$
\begin{aligned}
\nabla.\mathrm{B}(x,t) = 0, \qquad \varepsilon_0\nabla.\mathrm{E}(x,t) &= -\nabla.\mathrm{P}x,t) \\
\frac{\partial \mathrm{B}(x,t)}{\partial t} &= -\nabla \wedge \mathrm{E}(x,t) \\
\varepsilon_0 \frac{\partial \mathrm{E}(x,t)}{\partial t} = \varepsilon_0 c^2 \nabla \wedge \mathrm{B}(x,t) &- \left(\frac{d\mathrm{P}(x,t)}{\partial t} + \nabla \wedge \mathrm{M}(x,t)\right)
\end{aligned} \tag{7}
$$

which with the aid of (4) are seen to be the Maxwell equations.

If we are to obtain an equation of motion for the charge however, we shall have to construct an explicit form for the polarization fields $\mathrm{P}(x, t)$ and $\mathrm{M}(x, t)$. This may be done as follows: for any position, $\mathrm{R}(t)$, of the particle at a given instant in time t, we choose a curve, z, with an arbitrary starting point, r, to be discussed later, and ending at the point R. The paths to be specified are purely curves in space and have no time sequence attached to them; in order to obtain the equation of motion from the usual action principle one thus has to prescribe first the position of the particle as a function of time, and in addition, for each point a separate curve z. These latter curves must not therefore be confused with the actual path of the particle during its motion. We shall suppose that the polarization fields may be written in the form,

$$
\begin{aligned}
\mathrm{P}(x, t) &= e\int_r^{\mathrm{R}} dz\delta(z - x) \\
\mathrm{M}(x, t) &= e\int_r^{\mathrm{R}} (dz \wedge \dot{z})\delta(z - x)
\end{aligned} \tag{8}
$$

where the integrals are to be taken over the curves z described above. We shall leave until later the discussion of what restrictions (if any) on r are necessary for equations (4) and (8) to be consistent. We may now obtain that part of the lagrangian which depends on the particle variables by combining equations (3) and (8),

$$
\mathrm{L}' = \frac{1}{2}m\dot{\mathrm{R}}^2 + e\int_r^{\mathrm{R}} dz.\,\{\mathrm{E}(z, t) + \dot{z} \wedge \mathrm{B}(z, t)\} \tag{9}
$$

$$
= \frac{1}{2}m\dot{\mathrm{R}}^2 + \int_r^{\mathrm{R}} dz.\mathrm{F}(\dot{z}, z, t) \tag{10}
$$

$$
\equiv \mathrm{T} + \mathrm{V}
$$

in terms of the Lorentz force defined in equation (1). Thus the « potential energy » component, V, of the lagrangian for a charged particle moving in an electromagnetic field may be written as a line integral over the Lorentz force, the path being taken from some reference point r to the particle coordinate R.

The determination of the equation of motion for the particle is facilitated by the introduction of a summation convention for the components of vectors and tensors. Furthermore we shall make use of the antisymmetric unit tensor ε_{lmn} which has the property of vanishing if any two of its subscripts are equal, and alternates in value ($\pm$ 1) as its subscripts are permuted. We shall also need the relation [10],

$$\varepsilon_{tmn}\varepsilon_{tuv} = \delta_{mu}\delta_{nv} - \delta_{mv}\delta_{nv} \tag{11}$$

Since $\underline{\mathscr{L}}[\mathrm{T}] = -m\ddot{\underline{\mathrm{R}}}$, we wish to show that

$$\underline{\mathscr{L}}[\mathrm{V}] = \underline{\mathscr{L}}\left[\int_{\underline{r}}^{\mathrm{R}} d\underline{z}\,.\,\underline{\mathrm{F}}(\underline{z}, \dot{\underline{z}}, t)\right] = \underline{\mathrm{F}}(\underline{\mathrm{R}}, \dot{\underline{\mathrm{R}}}, t) \tag{12}$$

with $\underline{\mathrm{F}}$ given by equation (1). To begin with we shall only require that the fields $\underline{\mathrm{E}}(\underline{x}, t)$ and $\underline{\mathrm{B}}(\underline{x}, t)$ be differentiable. The total time derivative in $\underline{\mathscr{L}}$ is to be interpreted as,

$$\frac{d}{dt} = (\dot{\underline{\mathrm{R}}}\,.\,\underline{\nabla}_{\mathrm{R}}) + \frac{\partial}{\partial t} \tag{13}$$

of which a special case is

$$\dot{z}^n \equiv \frac{dz^n}{dt} = \dot{\mathrm{R}}^p(\partial z^n/\partial \mathrm{R}^p) \quad n, p = x, y, z \tag{14}$$

since the time variation of the path is due solely to the implicit time dependence of the endpoint $\underline{\mathrm{R}}(t)$ because of the assumed spatial character of the curve $\underline{z}$. The differentiation with respect to $\underline{\mathrm{R}}$ will be carried out under the integral sign and therefore we shall use

$$\frac{\partial}{\partial \mathrm{R}^p} = \left(\frac{\partial z^n}{\partial \mathrm{R}^p}\right)\frac{\partial}{\partial z^n} \tag{15}$$

Equations (14) and (15) may be simplified as follows: we introduce a parametric form for the path $\underline{z}=\underline{z}(s)$ with min $s=s_1$ giving $\underline{z}=\underline{r}$, and max $s=s_2$ giving $\underline{z} = \underline{\mathrm{R}}$; other values of s give points on the rest of the curve. But since z is only defined by the set of values of s there is no meaning to be associated with any variation of $\underline{z}$ (or $\underline{r}$, or $\underline{\mathrm{R}}$) that does not keep it on the curve. It is clear therefore that the only acceptable variations in the path lead to the result

$$\left(\frac{\partial z^n}{\partial \mathrm{R}^p}\right) = f(s)\delta_{np}; \quad f(s_1) = 0, \quad f(s_2) = 1; \tag{16}$$

for example, it is evident that if we start at $\underline{z} = \underline{\mathrm{R}}$, the only $d\underline{z}$ or $d\underline{\mathrm{R}}$ that we are allowed to introduce must be such that $d\underline{z}$ and $d\underline{\mathrm{R}}$ lie in the same direction (the tangent direction to the curve at this point) and thus $d\underline{z} \equiv d\underline{\mathrm{R}}$ there. The function $f(s)$ need not be specified in any more detail except that we shall suppose it to have a continuous first derivative in the subsequent analysis.

Thus if we apply $\underline{\mathscr{L}}$ to the path integral V,

$$\mathrm{V} = e\int_{s_1}^{s_2} ds(\partial z^r/\partial s)\,\{\,\mathrm{E}(\underline{z})^r + \varepsilon_{rsv} f(s)\dot{\mathrm{R}}^s\mathrm{B}(\underline{z})^v\,\} \tag{17}$$

we obtain the following derivatives;

$$(\nabla_{\mathrm{R}}\mathrm{V})^p = e\int_{s_1}^{s_2} ds f'(s)\mathrm{E}(\underline{z})^p + e\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{E}(\underline{z})^r/\partial z^p) + e\varepsilon_{rsv}\dot{\mathrm{R}}^s\nabla_{\mathrm{R}}^p\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)\mathrm{B}(\underline{z})^v \tag{18}$$

$$\left(\frac{\partial^2\mathrm{V}}{dt\partial\dot{\mathrm{R}}^p}\right) = e\varepsilon_{rpv}\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{B}(\underline{z})^v/\partial t) + e\varepsilon_{rpv}\dot{\mathrm{R}}^s\nabla_{\mathrm{R}}^s\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)\mathrm{B}(\underline{z})^v. \tag{19}$$

The terms in equations (18) and (19) obviously divide into two distinct types; those linear in the velocity $\dot{\underline{\mathrm{R}}}$, and the remainder, and so we consider these two groups separately. The contributions to $(\underline{\mathscr{L}}[\mathrm{V}])^p$ which are linear in $\dot{\underline{\mathrm{R}}}$ may be combined together to give

$$\begin{aligned} e\varepsilon_{vps}\dot{\mathrm{R}}^s\nabla_{\mathrm{R}}^r\int_{s_1}^{s_2} ds f(s)\,\{\,(\partial z^r/\partial s)\mathrm{B}(\underline{z})^v - (\partial z^v/\partial s)\mathrm{B}(\underline{z})^r\,\} \\ = e\varepsilon_{vps}\dot{\mathrm{R}}^s\int_{s_1}^{s_2} ds\,\{\,2f'(s)f(s)\mathrm{B}(\underline{z})^v + f(s)^2(\partial z^r/\partial s)(\partial \mathrm{B}(\underline{z})^v/\partial z^r) \\ - f(s)^2(\partial z^v/\partial s)(\underline{\nabla}.\underline{\mathrm{B}}(\underline{z}))\,\} \end{aligned} \tag{20}$$

after carrying out the $\underline{\nabla}_{\mathrm{R}}$ operation. The first two terms in (20) may be written as a perfect derivative

$$\partial(f(s)^2\mathrm{B}(\underline{z})^v)/\partial s$$

so that with the aid of the boundary values of $f(s)$ in equation (16), we may reduce equation (20) to the form

$$e(\dot{\underline{\mathrm{R}}} \wedge \underline{\mathrm{B}}(\underline{\mathrm{R}}))^p - e\int_{s_1}^{s_2} f(s)(d\underline{z} \wedge \dot{\underline{z}})^p(\underline{\nabla}.\underline{\mathrm{B}}(\underline{z})) \tag{21}$$

where we have written $d\underline{z}$ for $ds(\partial \underline{z}/\partial s)$.

The remaining contributions to $\underline{\mathscr{L}}[\mathrm{V}]$ are

$$e\int_{s_1}^{s_2} ds f'(s)\mathrm{E}(\underline{z})^p + e\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{E}(\underline{z})^r/\partial z^p) - e\varepsilon_{rpv}\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{B}(\underline{z})^v/\partial t); \tag{22}$$

using equation (11) we may write the second term in equation (22) as

$$e\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{E}(\underline{z})^r/\partial z^p)$$
$$= e\int_{s_1}^{s_2} ds f(s)(\partial \mathrm{E}(\underline{z})^p/\partial s) - e\varepsilon_{rpv}\varepsilon_{vmn}\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)(\partial \mathrm{E}(\underline{z})^n/\partial z^m)$$

so that equation (22) may bere written as,

$$e\int_{s_1}^{s_2} ds f'(s)\mathrm{E}(\underline{z})^p + e\int_{s_1}^{s_2} ds f(s)(\partial \mathrm{E}(\underline{z})^p/\partial s)$$
$$- e\varepsilon_{rpv}\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)\ \{\ (\partial \mathrm{B}(\underline{z})^v/\partial t) + \varepsilon_{vmn}(\partial \mathrm{E}(\underline{z})^n/\partial z^m)\ \}. \quad (23)$$

The first two terms now collect together into a perfect derivative and therefore (23) simplifies to

$$e\mathrm{E}(\underline{\mathrm{R}})^p - e\varepsilon_{rpv}\int_{s_1}^{s_2} ds f(s)(\partial z^r/\partial s)\ \{\ \partial \underline{\mathrm{B}}(\underline{z})/\partial t + \underline{\nabla} \wedge \underline{\mathrm{E}}(\underline{z})\ \}^v. \quad (24)$$

Thus collecting equations (21) and (24) together we obtain $\underline{\mathscr{L}}[\mathrm{V}]$ as,

$$\underline{\mathscr{L}}[\mathrm{V}] = e\ \{\ \underline{\mathrm{E}}(\underline{\mathrm{R}}) + \dot{\underline{\mathrm{R}}} \wedge \underline{\mathrm{B}}(\underline{\mathrm{R}})\ \}$$
$$- e\int_{s_1}^{s_2} ds f(s) d\underline{z} \wedge \{\ \partial \underline{\mathrm{B}}(\underline{z})/\partial t + \underline{\nabla} \wedge \underline{\mathrm{E}}(\underline{z}) + \dot{\underline{z}}(\underline{\nabla}.\underline{\mathrm{B}}(\underline{z}))\ \} \quad (25)$$

which only reduces to equation (12) *if* the integral term vanishes identically irrespective of the choice of path. Therefore in order to recover the Lorentz Force law for the equation of motion we must constrain the fields $\underline{\mathrm{E}}(\underline{x}, t)$ and $\underline{\mathrm{B}}(\underline{x}, t)$ to satisfy

$$\begin{aligned} \underline{\nabla}.\underline{\mathrm{B}}(\underline{x}, t) &= 0 \\ \partial \underline{\mathrm{B}}(\underline{x}, t)/\partial t &= -\ \underline{\nabla} \wedge \underline{\mathrm{E}}(\underline{x}, t) \end{aligned} \quad (26)$$

which are two of the Maxwell equations (7) (*).

In order to complete the proof that the lagrangian in equation (3) is a suitable expression for the description of the electrodynamics of charged particles, we must show that equations (4) and (8) are consistent. The total time derivative of $\underline{\mathrm{P}}(\underline{x})$ is easily obtained using (13) with the partial derivative omitted, and after an integration by parts this becomes

$$\frac{d\underline{\mathrm{P}}(\underline{x})^r}{dt} = e\dot{\mathrm{R}}^r\delta(\underline{z} - \underline{x}) f(s)\Big|_{s=s_1}^{s=s_2}$$
$$- e\dot{\mathrm{R}}^s\varepsilon_{prt}\varepsilon_{pus}(\partial/\partial x^t)\int_{s_1}^{s_2} ds f(s)(\partial z^u/\partial s)\delta(\underline{z} - \underline{x}); \quad (27)$$

(*) Note that in covariant notation these two equations combine together into the single equation,

$$f_{\mu\nu}{}^{,\rho} + f_{\nu\rho}{}^{,\mu} + f_{\rho\mu}{}^{,\nu} = 0$$

where $\underline{f}$ is the electromagnetic field tensor.

provided that the magnetization is defined as in (8) this equation is identical to the current equation (4). The divergence of the electric polarization field is

$$\underline{\nabla}.\underline{P}(\underline{x}, t) = - e\delta(\underline{z} - \underline{x}) \Big|_{s=s_1}^{s=s_2}$$
$$= - \rho(\underline{x}, t) + e\delta(\underline{x} - \underline{r}). \qquad (28)$$

The additional term $e\delta(\underline{x} - \underline{r})$ corresponds to an « image » charge fixed at the arbitrary point $\underline{r}$; since it is static it does not couple with the radiation field and so may be neglected in radiation problems (this is clear since it makes no appearance in the current equation (27)). To eliminate this term entirely one could for example choose $\underline{r}$ = spatial infinity, which although a natural choice for a single charge is a procedure that is quite analogous to imposing a gauge condition on the field potentials. We note however that if we have a collection of charged particles that is overall electrically neutral $\left(\sum_i e_i = 0\right)$, the corresponding term derived from equation (28), viz $\sum_i e_i\delta(\underline{x}-\underline{r})$ vanishes because of the electrical neutrality. In this situation which is the usual one in molecular physics, the choice of $\underline{r}$ is of no consequence and no restrictions need be imposed.

3. THE HAMILTONIAN

In order to obtain a hamiltonian description we use the momenta conjugate to the dynamical « coordinates » $\underline{R}$, $\phi(\underline{x}, t)$ and $\underline{A}(\underline{x}, t)$, in place of the lagrangian « velocities ». On introducing the field potentials into the lagrangian (3), one finds that the momentum density $\pi_0(\underline{x})$ conjugate to $\phi(\underline{x})$ vanishes formally. We have therefore a *degenerate* lagrangian system and may expect to find invariant relations amongst the dynamical variables. As before we shall follow Dirac's discussion of this type of problem [*1*], [*11*], [*12*]. For a finite dimensional system the momentum conjugate to the coordinate $\underline{R}$ is defined in the normal way to be $(\partial L/\partial \dot{\underline{R}})$; for an infinite dimensional field the momentum densities are the coefficients of $\delta\dot{\underline{R}}(\underline{x})$ in the variation of the lagrangian with respect to the velocities, $\delta_{vel}L = \int d^3x\underline{\pi}(\underline{x}).\delta\dot{\underline{R}}(\underline{x})$. From the lagrangian (3) we thus obtain,

$$\underline{p} \approx m\dot{\underline{R}} + \underline{Q}(\underline{B}) \qquad (29)$$

where,

$$\underline{\mathrm{Q}}(\underline{\mathrm{B}}) = e\int_{s_1}^{s_2} ds\, f(s)\underline{\mathrm{B}}(\underline{z}) \wedge (\partial \underline{z}/\partial s);$$

$$\underline{\pi}(\underline{x}) \approx -\ (\varepsilon_0 \underline{\mathrm{E}}(\underline{x}) + \underline{\mathrm{P}}(\underline{x})) \tag{30}$$

$$\pi_0(\underline{x}) \approx 0; \tag{31}$$

we have employed Dirac's « weak » equality sign $\approx$, because one of the canonical variables vanishes [*11*], [*12*]. In terms of the remaining canonical variables the hamiltonian may be written as

$$\mathscr{H} \approx (1/2\, m)(\underline{p} + \underline{\mathrm{Q}}(\underline{\mathrm{B}}))^2 + \frac{1}{2}\varepsilon_0^{-1}\int d^3\underline{x}\ \{\ (\underline{\pi}(\underline{x}) + \underline{\mathrm{P}}(\underline{x}))^2 + \varepsilon_0^2 c^2 \underline{\mathrm{B}}(\underline{x}).\underline{\mathrm{B}}(\underline{x})\ \} - \int d^3\underline{x}\phi(\underline{x})(\underline{\nabla}.\underline{\pi}(\underline{x})), \tag{32}$$

and the associated Poisson-brackets are assumed to be canonical,

$$[\mathrm{A}(\underline{x})^s, \pi(\underline{x}')^t] = \delta_{st}\delta(\underline{x} - \underline{x}') \tag{33}$$

$$[\phi(\underline{x}), \pi_0(\underline{x}')] = \delta(\underline{x} - \underline{x}') \tag{34}$$

$$[\mathrm{R}^s, p^t] \quad = \delta_{st}. \tag{35}$$

In order to achieve a consistent scheme we must ensure that equation (31) is true for all times, and this may be shown to imply the further condition

$$\underline{\nabla}.\underline{\pi}(\underline{x}) \approx 0 \tag{36}$$

which is the invariant relation that characterizes this formalism. The remainder of the argument follows exactly that given in ref. [*1*]; in order to make equation (36) a « strong » (*i. e.* ordinary) equality we introduce a supplementary condition on the vector potential, for example, the Coulomb gauge condition Div $\underline{\mathrm{A}}(\underline{x}) \approx 0$, and modify the definition of the Poisson-brackets according to Dirac's rule [*11*], [*12*]. The final result of these manipulations is the following hamiltonian scheme in which the redundant variables $\phi(\underline{x})$ and $\pi_0(\underline{x})$ no longer appear;

$$\mathscr{H}' = (1/2\, m)(\underline{p} + \underline{\mathrm{Q}}(\underline{\mathrm{B}}))^2 + \frac{1}{2}\varepsilon_0^{-1}\int d^3\underline{x}\ \{\ \underline{\pi}(\underline{x}).\underline{\pi}(\underline{x}) + 2\ \underline{\pi}(\underline{x}).\underline{\mathrm{P}}(\underline{x}) + \underline{\mathrm{P}}(\underline{x}).\underline{\mathrm{P}}(\underline{x}) + \varepsilon_0^2 c^2 \underline{\mathrm{B}}(\underline{x}).\underline{\mathrm{B}}(\underline{x})\ \} \tag{37}$$

$$\underline{\nabla}.\underline{\pi}(\underline{x}) = 0 \tag{38}$$

$$\underline{\nabla}.\underline{\mathrm{A}}(\underline{x}) = 0 \tag{39}$$

$$[\mathrm{R}^s, p^t]^* = \delta_{st} \tag{40}$$

$$[\mathrm{A}(\underline{x})^s, \pi(\underline{x}')^t]^* = \delta_{st}^{\perp}(\underline{x} - \underline{x}') \tag{41}$$

where $\delta_{st}^{\perp}(\underline{x})$ is the transverse delta function defined by Power [*13*].

A simple calculation shows that the Poisson-bracket of the momentum $\underline{\pi}(\underline{x})$ and the magnetic induction $\underline{B}(\underline{x})$ is

$$[\pi(\underline{x})^s, B(\underline{x}')^t]^* = -\varepsilon_{ust}(\partial/\partial x'_u)\delta(\underline{x} - \underline{x}') \tag{42}$$

and therefore we may identify the momentum $\underline{\pi}(\underline{x})$ with the electric field strength to within a constant factor.

$$\underline{\pi}(\underline{x}) = -\varepsilon_0 \underline{E}(\underline{x}). \tag{43}$$

Note that the Coulomb gauge condition is not essential to the argument leading to equations (37)-(41) in as much that any condition $g[\underline{A}(\underline{x})] \approx 0$ for which the Poisson-bracket $[g[\underline{A}(\underline{x})], \underline{\nabla}'.\underline{\pi}(\underline{x}')]$ is non-zero can be used here. However whereas an explicit gauge condition is an integral part of the usual hamiltonian scheme it is not difficult to see that here it is actually redundant. Since the vector potential only occurs in the hamiltonian through its Curl (the magnetic induction), the gauge condition (39) and the associated Poisson-bracket (41) may be dropped, and instead we may write the hamiltonian purely in terms of the canonical variables $\{ \underline{R}, \underline{p} \}$ and the electromagnetic field variables $\{ \underline{E}(\underline{x}), \underline{B}(\underline{x}) \}$,

$$\mathcal{H}' = (1/2\,m)(\underline{p} + \underline{Q}(\underline{B}))^2 - \int d^3x\underline{P}(\underline{x}).\underline{E}(\underline{x})^{\perp} + \frac{1}{2}\varepsilon_0^{-1}\int d^3x\underline{P}(\underline{x}).\underline{P}(\underline{x})$$
$$+ \frac{1}{2}\varepsilon_0 \int d^3\underline{x}\, \{ \underline{E}(\underline{x})^{\perp}.\underline{E})x)^{\perp} + c^2\underline{B}(\underline{x}).\underline{B}(\underline{x}) \} \tag{44}$$

together with the following Poisson-brackets,

$$[R^s, p^t] = \delta_{st} \tag{45}$$

$$[E(\underline{x})^s, B(\underline{x}')^t] = \varepsilon_0^{-1}\varepsilon_{ust}(\partial/\partial x'_u)\delta(\underline{x} - \underline{x}'). \tag{46}$$

The formal quantization of this canonical system is immediate and leads to a quantum theory in the Heisenberg representation.

It may be remarked that in the usual theory of the electrodynamics of a charged particle one obtains an invariant relation which contains both field and particle variables [*14*], [*15*]

$$\underline{\nabla}.\underline{\pi}(\underline{x}) + \rho(\underline{x}) = 0. \tag{47}$$

As a result the Poisson-brackets of the particle momentum and the vector potential with the field momentum, $\underline{\pi}(\underline{x})$, are gauge dependent. Under a gauge transformation however these dynamical variables and their Poisson-brackets change in such a way that the kinetic momentum $(\underline{p} - e\underline{A}(\underline{R}))$ is a gauge-invariant quantity. This behaviour is to be contrasted with the simplicity of the present formulation.

When more than one charge is considered, the hamiltonian scheme (44)-(46) may be generalized without difficulty. It suffices to give the particle variables an appropriate index and to introduce a summation over all particles; if one wishes, different arbitrary origins $\underline{r}_\alpha$ can be associated with subsets of the particles, so that one can bring into the formalism the notion of well defined atomic systems through the individual atomic polarization fields,

$$\underline{\mathrm{P}}(\underline{x})^{\mathrm{Total}} = \sum_{\alpha}^{\substack{\text{all}\\ \text{atoms}}} \underline{\mathrm{P}}(\alpha : \underline{x})$$

$$\underline{\mathrm{P}}(\alpha : \underline{x}) = \sum_i e_{\alpha i} \int_{\underline{r}_\alpha}^{\underline{\mathrm{R}}_{\alpha i}} d\underline{z}\,\delta(\underline{z} - \underline{x}). \tag{48}$$

It is understood here that a curve $\underline{z}_i$ is to be defined for each particle i. The relationship between the term $\int d^3x\underline{\mathrm{P}}(\underline{x}).\underline{\mathrm{P}}(\underline{x})$ in the hamiltonian and the instantaneous Coulomb interaction energies,

$$\mathrm{V}^{\mathrm{COU}} = \sum_{\alpha,\beta}\sum_{i,j} \frac{e_{\alpha i}e_{\beta j}}{4\,\pi\varepsilon_0\,|\,\underline{\mathrm{R}}_{\alpha i} - \underline{\mathrm{R}}_{\beta i}\,|}, \tag{49}$$

in the many particle case has been discussed elsewhere [*15*]. It is most important that the Coulomb energies are found in the contribution from the longitudinal part of the polarization field, *i. e.* $\mathrm{V}^{\mathrm{COU}} \propto \int d^3x\underline{\mathrm{P}}(\underline{x})^{||}.\underline{\mathrm{P}}(\underline{x})^{||}$ rather than in the total integral, $\int d^3x\underline{\mathrm{P}}(\underline{x}).\underline{\mathrm{P}}(\underline{x})$. In the case of a single atom interacting with radiation one puts $\int d^3x\underline{\mathrm{P}}(\underline{x})^{\perp}.\underline{\mathrm{P}}(\underline{x})^{\perp}$ (according to the usual quantum mechanical perturbation theory arguments this is an « atomic » self-energy term) into the perturbation part of the hamiltonian, V, so that one can write $\mathscr{H}' = \mathrm{H}^{\mathrm{RAD}} + \mathrm{H}^{\mathrm{ATOM}} + \mathrm{V}$. This decomposition is *not* extended when the formalism is generalized to describe interactions involving more than one atom; the entire integral $\sum_{\alpha\neq\beta}\int d^3x\underline{\mathrm{P}}(\alpha : \underline{x}).\underline{\mathrm{P}}(\beta : \underline{x})$ is regarded as a contribution to the perturbation operator V. It then follows that interactions between different atoms can be described in terms of purely retarded transverse radiation transfers (there are no *explicit* intermolecular Coulomb energies in the hamiltonian) and this often leads to a simplified form of perturbation theory in comparison with the conventional Coulomb gauge theory in which static Coulomb terms may give rise to difficulties [*16*], [*17*].

Finally we show how the perturbation operators, for example

$\int d^3\underline{x}\underline{P}(\underline{x}).\underline{E}(\underline{x})^\perp$ may be transformed to the familiar multipolar form; with the aid of (48) we may write for one atom

$$V = -\sum_i e_i \int_{\underline{r}}^{\underline{R}_i} d\underline{z}.\underline{E}(\underline{z})^\perp. \tag{50}$$

In the long wavelength limit $\underline{E}(\underline{z})$ is approximately constant over the range of integration (roughly the extent of the electron distribution in the atom) so that it may be moved to the left of the integral sign, and (50) reduces to

$$V \sim -\sum_i e_i \underline{E}(\underline{r}).\int_{\underline{r}}^{\underline{R}_i} d\underline{z} \equiv -\underline{d}.\underline{E}(\underline{r}) \tag{51}$$

where $\underline{d}$ is the usual electric dipole operator. Higher order multipole operators are generated by expanding the integrand in (50) about $\underline{r}$ as a Taylor series and integrating term by term.

4. DISCUSSION

In the previous sections we have shown that the lagrangian in equation (3) which is expressed in terms of the electromagnetic field variables and the material polarization fields, leads to the expected equations of motion for the charged particle (the Lorentz Force Law) and the electromagnetic field (the Maxwell equations) when supplemented by the definitions in equation (8). Starting from this lagrangian we have constructed an equivalent classical hamiltonian description, equations (44)-(46), in which the dynamical variables are the particle's position $\underline{R}$ and momentum $\underline{p}$, and the transverse radiation field variables $\underline{E}(\underline{x})^\perp$ and $\underline{B}(\underline{x})$. The possibility of achieving this explicit separation of the radiation field from the longitudinal electric field is apparently a consequence of the choice of the curves $\underline{z} = \underline{z}(s)$ which have no time dependence, and are thus purely spatial in character. If one were to attempt a relativistic theory based on the formalism given above, it would be necessary to use curves in space-time if the theory were to be manifestly covariant. We shall not however pursue a covariant theory here, and shall only refer to the formulations of quantum electrodynamics proposed by Mandelstam [*18*] and Goldberg [*19*]. The combination of this hamiltonian scheme with the usual perturbation theory methods provides an extremely convenient formalism for discussing the interactions of molecules with radiation, and it is in molecular physics that this formalism may be expected to find its most valuable applications [*1*], [*13*], [*16*].

Although we have eliminated the field potentials, the interaction terms are non-local, and it is this non-locality which enables us to describe the

Bohm-Aharonov effect with the hamiltonian (44). Bohm and Aharonov consider the scattering of an electron beam by a uniform magnetic field due to a solenoid of radius a, which is perpendicular to the plane of the beam, and show that quantum mechanics (but not classical mechanics) predicts the existence of a novel interference effect even though the electrons never pass through a region of non-zero magnetic induction [8], [9], [20]. Inside the solenoid the field has magnitude B_0 whereas outside the solenoid the field vanishes. The perturbation operator required comes from the term $(\underline{p} + \underline{Q}(\underline{B}))^2/2m$ in the hamiltonian, and so we must evaluate the integral $\underline{Q}(\underline{B})$

$$\underline{Q}(\underline{B}) = \int_{s_1}^{s_2} ds\, f(s)\underline{B}(\underline{z}) \wedge (\partial \underline{z}/\partial s). \tag{52}$$

It is natural to use cylindrical coordinates (R, x, θ) since then only Q_θ is non-zero for the experimental configuration described above. Choosing the integration path as the straight line from the centre of the solenoid to the particle coordinate, $\underline{z} = s\underline{R}$ $(0 \leqslant s \leqslant 1)$, we find $f(s) = s$, $(\partial \underline{z}/\partial s) = \underline{R}$ and

$$Q_\theta = eRB_0 \int_0^1 ds\, sb(s) \tag{53}$$

where

$$b(s) = \begin{cases} 1, \text{ all } s & R \leqslant a \\ H(a/R - s) & R > a \end{cases} \tag{54}$$

($H(x)$ is Heaviside's step function) describes the cut-off in the field at the surface of the solenoid. Thus

$$Q_\theta = \begin{cases} \dfrac{1}{2} eRB_0 & R \leqslant a \\ \dfrac{1}{2} eB_0 a^2/R & R > a \end{cases} \tag{55}$$

and so we obtain exactly the same Schrödinger equation as that discussed by Bohm and Aharonov in their original article [8].

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