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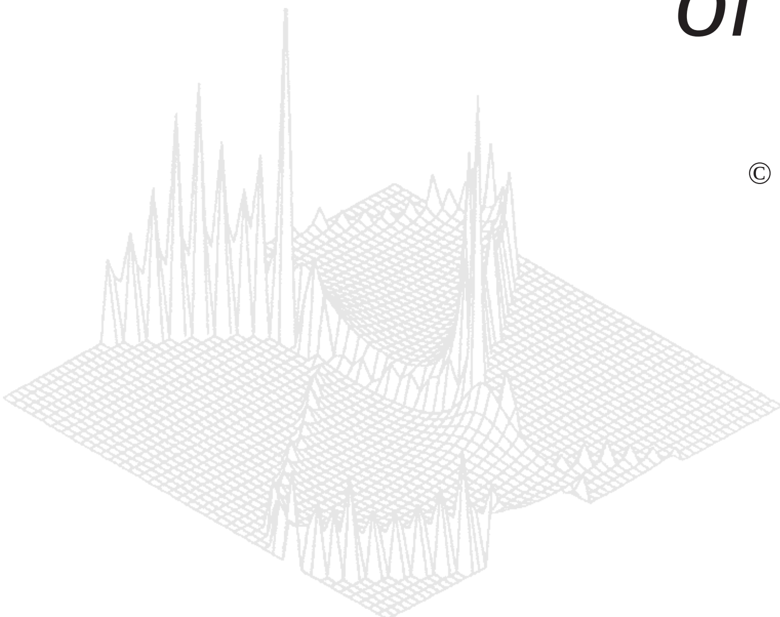

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Gauge Explicit Quantum Mechanics and Perturbation Theory

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Abstract

A version of quantum and statistical mechanics, including perturbation theory, is described in which explicit electromagnetic gauge arbitrariness is maintained at every stage. Any gauge may be used for a calculation provided that the wave equation operator is gauge invariant.

1. Introduction

In classical electrodynamics it is well known (see for example Cohen-Tannoudij *et al*. 1977; Healy 1982; Craig and Thirunamachandran 1984; Doughty 1990) that if the vector and scalar electromagnetic potentials $\mathbf{A}$ and ϕ are transformed to $\mathbf{A}_\chi$ and ϕ_χ where

$$\mathbf{A}_\chi = \mathbf{A} + \nabla\chi \quad \text{and} \ \phi_\chi = \phi - \partial\chi/\partial t\,, \tag{1}$$

then the electromagnetic fields $\mathbf{B}$ and $\mathbf{E}$ given by

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \text{and} \ \mathbf{E} = -\nabla\phi - \partial\mathbf{A}/\partial t \tag{2}$$

remain unchanged. The arbitrary non-operator scalar field $\chi(\mathbf{r}, t)$, which is a continuously differentiable single valued function of position $\mathbf{r}$ and time t as are the fields and potentials, is known as the gauge function and the transformation as a gauge transformation.

In quantum mechanics it is also known that if the wavefunction Ψ of the system that is transformed becomes

$$\Psi_\chi = \Psi_0 \exp(\mathrm{i}e\chi/\hbar)\,, \tag{3}$$

where e is the electric charge of the particle, then the transformed Hamiltonian H_χ (which involves $\mathbf{A}_\chi$ and ϕ_χ) and wavefunction Ψ_χ will obey a time-dependent Schrödinger wave equation of the same form as the untransformed one involving $\mathbf{A}$ and ϕ. Consider the Schrödinger equation $S_0\,\Psi_0 = 0$ for a particle of rest mass m moving in potentials $\mathbf{A}$ and ϕ, where the Schrödinger wave equation operator

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is $S_0 = H_0 - i\hbar\partial/\partial t$ and H_0 is the non-relativistic Hamiltonian written in the gauge with $\chi = 0$ which is denoted by the subscript 0:

$$H_0 = (\mathbf{p} - e\mathbf{A})^2/2m + e\phi\,, \tag{4}$$

and $\mathbf{p}$ is the canonical momentum operator $\mathbf{p} = -i\hbar\nabla$. This transforms into $S_\chi\,\Psi_\chi = 0$, where the operator and wavefunction are obtained from transformations (1) and (3) because the gradient operator acting on the phase of the transformed wavefunction produces a term that cancels that coming from the $e\nabla\chi$ term and the time derivative operator cancels the $e\partial\chi/\partial t$ term. The gauge function must be real so that physical quantities such as charge and current densities remain unchanged. The property of the wave equation of being invariant in form under a gauge transformation is known as gauge covariance. In the remainder of the paper a subscript is attached to operators and wavefunctions to denote the value of the gauge function associated with them.

The freedom to specify χ may be used to simplify a calculation. For example, in the Lorentz gauge the condition $\nabla\boldsymbol{.}\mathbf{A} + c^{-2}\partial\phi/\partial t = 0$ is imposed by requiring χ to obey the inhomogeneous wave equation. This has the effect of separating the electrodynamic equations of motion for $\mathbf{A}$ and ϕ. The interaction of radiation with atoms and molecules is most effectively dealt with in the Coulomb gauge with $\nabla\boldsymbol{.}\mathbf{A} = 0$ (Craig and Thirunamachandran 1984) or in the dipole gauge (Goppert-Mayer 1931). For a discussion of many other gauges see Leibbrandt (1987). However, even after such a gauge transformation a degree of gauge arbitrariness will remain. The object of the present paper is to describe the formal structure of quantum mechanics and perturbation theory when full gauge arbitrariness is preserved manifestly at every stage. For the purpose of this paper quantum mechanics is taken to be the wave mechanics of Schrödinger. Because, as has been known almost since its inception, quantum mechanics is gauge invariant, it is necessary that at the end of any calculation all observable quantities must be independent of gauge and so must agree with the results of a conventional calculation which might assume, for example, simply that $\chi = 0$.

The question of how probability amplitudes may be defined in the presence of a time-dependent gauge function was addressed by Yang (1976), following a comment on the matter by Lamb (1952), and contributions to this and allied issues were made subsequently by many authors: see for example Kobe (1978, 1984), Power and Thirunamachandran (1978), Aharonov and Au (1981, 1983), Yang (1981), Feuchtwang *et al.* (1982), Haller (1984), Schlicher *et al.* (1984), Power (1989) and Healy (1988). Some of these authors, following Yang (1976), suggested that it is possible to define eigenvalues and eigenfunctions for time-dependent gauge functions through the equation $H(t)\,\Psi(t) = E(t)\,\Psi(t)$. Although this approach is valuable for dealing with adiabatic processes, see for example Griffiths (1994), its use here is precluded by the arbitrarily fast time variations of the gauge function. We argue that the time-dependent Schrödinger equation must be used throughout and that it is only possible to define basis states formally in terms of fields that are time *independent* and that these basis states will be time *dependent.*

In Section 2 of this paper we show how wavefunctions and basis functions may be defined for a wave equation in which the gauge is arbitrary. In Section 3 we discuss the properties of operators in different gauges and, in Sections 4 and 5, time-independent perturbation theory and statistical mechanics. In Section 6 time-dependent perturbation theory and probability amplitudes are examined.

2. Basis Functions

We consider the Schrödinger wave equation $S_\chi \Psi_\chi = 0$ for a single particle in an arbitrary gauge χ which, written explicitly, is

$$[\{\mathbf{p} - e(\mathbf{A} + \nabla\chi)\}^2/2m + e(\phi - \partial\chi/\partial t) - \mathrm{i}\hbar\partial/\partial t]\Psi_\chi(\mathbf{r},\, t) = 0\,. \tag{5}$$

We note that due to the presence of χ the Hamiltonian, which is the sum of the first two operators, is time dependent even when the potentials are static. In this circumstance the wavefunction cannot be separated into the product of a time-dependent part and a space dependent part and so the time-dependent wave equation must be used throughout. However, if $\mathbf{E}$ and $\mathbf{B}$ have no time dependence it follows from equations (2) that it is always possible to find a gauge in which the potentials have no time dependence either and are functions of $\mathbf{r}$ alone, any time dependence residing solely in the gauge function. We call these potentials $\mathbf{A}^0(\mathbf{r})$ and $\phi^0(\mathbf{r})$, they are functions of the charges and currents that are the sources of the fields. To give a concrete example consider the potentials due to a long cylindrical solenoid of radius R parallel to the z axis containing a steady magnetic flux Φ. The potentials in the time-independent gauge that we require are found from Stoke's theorem to be $A^0_\theta = \Phi r/2\pi R^2$ for $r \le R$ and $A^0_\theta = \Phi/2\pi r$ for $r \ge R$ with $A^0_r = A^0_z = \phi^0 = 0$ everywhere, where $(r,\, \theta,\, z)$ are the cylindrical coordinates (see e.g. Griffiths 1994). Other gauges may be constructed by adding various derivatives of a gauge function but if this is time dependent a time dependence of the potentials may be introduced and they will not be appropriate for our present purpose.

To solve (5) with static potentials we temporarily set χ to zero. This gives

$$[(\mathbf{p} - e\mathbf{A}^0)^2/2m + e\phi^0]\Psi_0(\mathbf{r},\, t) = \mathrm{i}\hbar(\partial/\partial t)\,\Psi_0(\mathbf{r},\, t)\,. \tag{6}$$

Since the operator on the left-hand side is now independent of time the wavefunction may be factored into a space-dependent part $\psi(\mathbf{r})$ and a time-dependent part. These separate in the usual way to give

$$\Psi_{0,n}(\mathbf{r},\, t) = \psi_n(\mathbf{r})\exp(-\mathrm{i}E_n\, t/\hbar)\,, \tag{7}$$

with E_n and $\psi_n(\mathbf{r})$ given by the eigenvalue equation

$$[(\mathbf{p} - e\mathbf{A}^0)^2/2m + e\phi^0]\psi_n(\mathbf{r}) = E_n\,\psi_n(\mathbf{r})\,, \tag{8}$$

whose solutions are assumed to be known. They are complete and orthonormal because the operator is Hermitian. We are now able to restore gauge dependence by appealing to (3) which gives

$$\Psi_{\chi,n}(\mathbf{r},\, t) = \psi_n(\mathbf{r})\exp[\mathrm{i}(e\chi - E_n\, t)/\hbar]\,. \tag{9}$$

We emphasise that we have not fixed the gauge (at a value of zero) in the preceding process. It may be verified by substitution that (9) is a solution of (5) with the time-independent potentials $\mathbf{A}^0$ and ϕ^0. The $\Psi_{\chi,n}$ are time-dependent solutions of the wave equation for time-independent fields. Their space and time dependences are arbitrarily and inextricably linked by the gauge function. Any linear combination of them $\Psi_\chi(\mathbf{r},\, t) = \sum_n a_n\, \Psi_{\chi,n}(\mathbf{r},\, t)$, where the a_n are independent of time is also a solution of (5) with static fields. In this situation the gauge explicit probability amplitude for the system to be in state m at time t is defined to be the projection of state m onto the wavefunction $\Psi_\chi(\mathbf{r}, t)$

$$\int \Psi^*_{\chi,\mathrm{m}}(\mathbf{r},\, t)\, \Psi_\chi(\mathbf{r},\, t)\, \mathrm{d}\mathbf{r}\,,$$

which is equal to a_m due to the orthonormality of the $\psi_n(\mathbf{r})$ and so is independent of gauge and, in the present case, of time. The probability of the system being in a particular state m is therefore equal to $|a_m|^2$. If the operator on the left side of (8) is the exact Hamiltonian operator the solutions are exact. If it is only part of the total Hamiltonian then the solutions form a basis set with which perturbation theory may be carried out.

3. Operators and Matrix Elements

An operator O_0 in the gauge with $\chi = 0$ is, in general, a function of the potentials, i.e. $O_0 = O_0(\mathbf{A}, \phi)$. The operator O_χ in gauge χ is defined by the relation $O_\chi(\mathbf{A},\, \phi) = O_0(\mathbf{A} + \nabla\chi,\, \phi - \partial\chi/\partial t)$. We define a gauge *independent* operator I to be one that is unchanged by a gauge transformation so that $I_\chi(\mathbf{A},\, \phi) = I_0(\mathbf{A} + \nabla\chi,\, \phi - \partial\chi/\partial t) = I_0(\mathbf{A},\, \phi)$. An operator such as $\mathbf{r}$ or $\mathbf{p}$ that does not depend explicitly on the potentials is gauge independent.

That the Schrödinger equation (5) $S_\chi\, \mathrm{e}^{\mathrm{i}e\chi/\hbar}\, \Psi_0 = 0$ transforms unitarily to $S_0\, \Psi_0 = 0$ under a gauge transformation is seen to require that

$$S_\chi = \mathrm{e}^{\mathrm{i}e\chi/\hbar}\, S_0\, \mathrm{e}^{-\mathrm{i}e\chi/\hbar}\,. \tag{10}$$

An operator that satisfies such a relation is said to be gauge *invariant.* It is clear that any operator O that has the functional form $O_0 = O_0(\mathbf{r},\, t,\, \mathbf{p}-e\mathbf{A},\, \mathrm{i}\hbar\partial/\partial t - e\phi)$ will be gauge invariant if the operator can be expanded in sums of powers of its arguments. We now see that the matrix elements of a gauge invariant operator O are independent of gauge. By using equations (3) and (10) it follows that

$$\langle\Psi_{\chi,m}|O_\chi|\Psi_{\chi,n}\rangle = \langle\psi_m(\mathbf{r})\exp(\mathrm{i}E_m\, t/\hbar)|O_0|\psi_n(\mathbf{r})\exp(-\mathrm{i}E_n\, t/\hbar)\rangle\,. \tag{11}$$

If O does not contain a time derivative the matrix element is simply

$$\langle\Psi_{\chi,m}|O_\chi|\Psi_{\chi,n}\rangle = \exp[(\mathrm{i}(E_m - E_n)t/\hbar] \int \psi^*_m(\mathbf{r})\, O_0\, \psi_n(\mathbf{r})\, \mathrm{d}\mathbf{r}\,. \tag{12}$$

Expectation values, which are given by the diagonal elements, are independent of time. It is apparent that an operator that represents a physical observable is required to be gauge invariant but need not be gauge independent. One important operator that is neither gauge invariant nor gauge independent is the semiclassical Hamiltonian. From examination of equations (4) and (5) it is seen that

$$H_\chi = \mathrm{e}^{\mathrm{i}e\chi/\hbar}\, H_0\, \mathrm{e}^{-\mathrm{i}e\chi/\hbar} - e\partial\chi/\partial t\,, \tag{13}$$

and its matrix elements are

$$\langle\Psi_{\chi,m}|H_\chi|\Psi_{\chi,n}\rangle = (E_n - e\partial\chi/\partial t)\delta_{m,n}\,, \tag{14}$$

due to the orthonormality of the $\psi_n(\mathbf{r})$, where δ is the Kronecker delta. But although there is a gauge dependent shift of individual energies, interpreted here as the eigenvalues of the Hamiltonian, energy *differences* remain unchanged so spectroscopy is gauge independent. This gauge variance is the price that must be paid for requiring the electromagnetic fields to be externally prescribed; a quantum electrodynamical calculation gives a Hamiltonian that is gauge invariant.

We have seen that the Schrödinger operator S is gauge invariant but its Hamiltonian H is not. Similarly the Dirac operator given by

$$D_0 = c\boldsymbol{\alpha}\,.\,(\mathbf{p} - e\mathbf{A}) + \beta mc^2 + e\phi - \mathrm{i}\hbar\partial/\partial t\,, \tag{15}$$

where c is the speed of light and β and the $\boldsymbol{\alpha}$ are the four 4×4 Dirac matrices, is gauge invariant, but the Dirac Hamiltonian itself, $D_0 + \mathrm{i}\hbar\partial/\partial t$, is not either. The derivation of the solutions of the Dirac equation with time-independent fields goes exactly as in Section 2, except that the eigensolutions are those of (8) with $[c\boldsymbol{\alpha}\,.\,(\mathbf{p} - e\mathbf{A}^0) + \beta mc^2 + e\phi^0]$ as the operator on the left-hand side. The arguments given in this paper so far therefore hold for particles described by the Dirac equation and its various non-relativistic approximations (Foldy and Wouthuysen 1950; Frohlich and Studer 1993) all of which are gauge invariant.

In the discussion above it is important to distinguish the notions of gauge invariance, defined by (10), and gauge independence, which means that the quantity concerned does not change when the gauge function is changed. For example the position operator $\mathbf{r}$ is both gauge independent and gauge invariant, the canonical momentum operator $\mathbf{p}$ is gauge independent but not gauge invariant and the Hamiltonian is neither gauge independent nor gauge invariant.

4. Time-independent Perturbations

If the potentials in equations (5) or (15) are separated into two parts so that $\mathbf{A} \to \mathbf{A}^0 + \mathbf{A}^1$ and $\phi \to \phi^0 + \phi^1$ then the wave equations may be written formally as

$$[H_\chi^0 + V_\chi - \mathrm{i}\hbar\partial/\partial t]\,\Psi_\chi(\mathbf{r}, t) = 0\,, \tag{16}$$

where for the Dirac Hamiltonian $H_\chi^0 = c\boldsymbol{\alpha}\,.\,\{\mathbf{p} - e(\mathbf{A}^0 + \nabla\chi)\} + \beta mc^2 + e(\phi^0 - \partial\chi/\partial t)$and $V_\chi = -ec\boldsymbol{\alpha}.\mathbf{A}^1 + e\phi^1$, the latter being independent of χ. For the Schrödinger Hamiltonian the two operators are $H_\chi^0 = \{\mathbf{p} - e(\mathbf{A}^0 + \nabla\chi)\}^2/2m + e(\phi^0 - \partial\chi/\partial t)$ and $V_\chi = -\mathbf{A}^1\,.\,\{\mathbf{p} - e(\mathbf{A}^0 + \nabla\chi)\}e/m + e^2(\mathbf{A}^1)^2/2m + \mathrm{i}e\hbar(\nabla\,.\,\mathbf{A}^1)/2m + e\phi^1$, which does depend on χ. However, it is to be noted that in both cases the perturbation V_χ satisfies the relation $V_\chi = \exp(-\mathrm{i}e\chi/\hbar)\, V_0 \exp(-\mathrm{i}e\chi/\hbar)$; in the case of the Dirac Hamiltonian trivially, in the case of the Schrödinger Hamiltonian because the operator $\mathbf{p}$ generates the $e\nabla\chi$ term from the phase factor that contains the gauge function. In both cases H_χ^0 has the form of an unperturbed Hamiltonian in the gauge χ. For a perturbative approach to be viable it is necessary for the matrix elements associated with V_0 to be smaller than those associated with ${H_0}^0$.

If $\mathbf{A}^1$ and ϕ^1 are independent of time, then V_0 is also, so instead of the eigensolutions $\psi_n(\mathbf{r})$ and E_n being determined by (8): ${H_0}^0\psi_n = E_n\psi_n$, where ${H_0}^0$ is the unperturbed Hamiltonian in the $\chi = 0$ gauge, they will be determined by the new eigenvalue equation $({H_0}^0 + V_0)\psi'_n = E'_n\,\psi'_n$. This may be solved for the E'_n and ψ'_n in terms of the E_n and ψ_n by the standard methods of time-independent perturbation theory. New gauge dependent wavefunctions may then be constructed with the primed quantities by means of (9) and the expectation values of operators that represent physical quantities may be evaluated.

But there is one condition that must be satisfied. From (10) the wave equation operator $(H^0 - \mathrm{i}\hbar\partial/\partial t)$ is required to be gauge invariant. Therefore for it to remain so when an extra term V is added this extra term must satisfy the relation $V_\chi = \exp(\mathrm{i}e\chi/\hbar)\,V_0\exp(-\mathrm{i}e\chi/\hbar)$. To illustrate the importance of this requirement, the spin–orbit interaction is sometimes incorrectly taken to be of the form $\xi(\mathbf{r})\,\mathbf{l.s}$ where $\mathbf{l} = \mathbf{r}\times\mathbf{p}$. However, the correct form of this interaction is gauge invariant as it involves the gauge invariant quantities $\mathbf{E}, (\mathbf{p} - e\mathbf{A})$ and $\mathbf{s}$ (Frohlich and Studer 1993) and it is in this form that it must be used as a perturbation.

Generally, the quantities under the control of an experimenter are the fields $\mathbf{E}$ and $\mathbf{B}$ which are determined by the placement of electrodes and magnets. The potentials cannot be controlled in this way. Therefore when the fields are considered to be applied externally and their operator nature is ignored an appropriate form of perturbation to use is the derivative of the Hamiltonian with respect to these fields:

$$V = \delta\mathbf{E}\,.\,\partial H/\partial\mathbf{E} + \delta\mathbf{B}\,.\,\partial H/\partial\mathbf{B} + \text{higher terms}\,, \tag{17}$$

where the partial derivative with respect to a vector means the gradient with respect to that vector and $\delta\mathbf{E}$ and $\delta\mathbf{B}$ are small variations of these fields. This form of perturbation fits readily into thermodynamic perturbation theory (Stewart 1996*a*). If, for example, the potentials corresponding to static uniform fields $\mathbf{E}$ and $\mathbf{B}$ are taken to be $\phi = -\mathbf{E}\,.\,(\mathbf{r} - \mathbf{R})$ and $\mathbf{A} = \mathbf{B}\times(\mathbf{r} - \mathbf{R})/2$, the origin of the potentials being at $\mathbf{R}$, then from (4), $-\partial H/\partial\mathbf{E} = e(\mathbf{r} - \mathbf{R})$ the electric dipole moment. The term $\mathbf{E}\,.\,\mathbf{R}$ in the Hamiltonian gives rise to a shift of all energy levels and is unobservable.

The derivative of H with respect to the ith component of $\mathbf{B}$ is

$$\partial H/\partial B_i = \sum_j(\partial H/\partial A_j)(\partial A_j/\partial B_i)\,. \tag{18}$$

The quantity $\partial H/\partial\mathbf{A} = ec\boldsymbol{\alpha}$ for the Dirac equation and is given for the Schrödinger equation by $H(\mathbf{A} + \delta\mathbf{A}) - H(\mathbf{A}) = -\delta\mathbf{A}\,.\,(\mathbf{p} - e\mathbf{A})e/m$ for fields with $\nabla\,.\,\mathbf{A} = 0$. For a uniform magnetic field, $\partial A_i/\partial B_j = \sum_k \epsilon_{ijk}\,r'_k/2$, where the Levi-Civita unit tensor ϵ_{ijk} is zero if any two of the subscripts are the same, unity if they are in cyclic order and zero otherwise, and $\mathbf{r}' = \mathbf{r} - \mathbf{R}$.

Accordingly

$$\frac{\partial H}{\partial B_{\mathrm{x}}} = \tfrac{1}{2}\left(y'\,\frac{\partial H}{\partial A_{\mathrm{z}}} - z'\,\frac{\partial H}{\partial A_{\mathrm{y}}}\right), \tag{19}$$

etc. and so $-\partial H/\partial\mathbf{B} = \mathbf{r}' \times \boldsymbol{\alpha} ce/2$ for the Dirac Hamiltonian and $\mathbf{r}' \times (\mathbf{p} - e\mathbf{A})e/2m$ for the Schrödinger Hamiltonian. The latter is the expression for the orbital magnetic moment operator in non-relativistic quantum mechanics, the first and second terms representing the paramagnetic and diamagnetic contributions respectively. Since the paramagnetic and diamagnetic terms are not individually gauge invariant they are not observable individually, only the sum of them is (Stewart 1996*b*). The expression for $\partial H/\partial\mathbf{B}$ involves a cross product with $(\mathbf{r} - \mathbf{R})$. The term containing $\mathbf{R} \times \boldsymbol{\alpha}$ or $\mathbf{R} \times (\mathbf{p} - e\mathbf{A})$ is the cross product of the constant vector $\mathbf{R}$ with an operator that represents a drift current. By Maxwell's equations a drift current is inconsistent with a uniform magnetic field and consequently in this case the expectation value of $\partial H/\partial\mathbf{B}$ is required to be independent of $\mathbf{R}$. In this derivation the derivatives of the Hamiltonian have been calculated in the gauge with $\chi = 0$. With general gauge $\partial H/\partial\mathbf{B}$ is unchanged for the Dirac Hamiltonian, for the Schrödinger Hamiltonian it becomes $\mathbf{r}' \times (\mathbf{p} - e\mathbf{A} - e\nabla\chi)e/2m$; $\partial H/\partial\mathbf{E}$ is unchanged. These derivatives of the Hamiltonian are evidently gauge invariant and so are observable.

5. Statistical Mechanics

We assume that the behaviour of an assembly of particles i, j, etc. is governed by the Schrödinger equation $S\Psi(\mathbf{r}_i, \mathbf{r}_j, t) = 0$, where $S = H - \mathrm{i}\hbar\partial/\partial t$ and $H(\mathbf{r}_i, \mathbf{r}_j, t)$ is a non-relativistic Hamiltonian consisting of the sum of single-particle terms, for example as in (5), plus an interaction term involving the spatial coordinates of two or more particles. Because the latter is gauge invariant as it depends only on coordinates, the many particle Schrödinger operator will be gauge invariant too. The gauge function Ξ of the many body wavefunction is the sum of the individual gauge functions of the particles: $\Xi(\mathbf{r}_i, \mathbf{r}_j, t) = \sum_i \chi(\mathbf{r}_i, t)$ so that $\Psi_\Xi(\mathbf{r}_i, \mathbf{r}_j, t) = \Psi_0(\mathbf{r}_i, \mathbf{r}_j, t)\exp(\mathrm{i}e\Xi/\hbar)$. For the time-independent fields appropriate for thermodynamics (or more correctly thermostatics) the solutions of the wave equations are analogous to those of the single particle situation except that the eigensolutions of (8) are now those for the many particle rather than the single particle Hamiltonian and χ becomes Ξ.

Consider the quantity $\mathrm{Tr}(\mathrm{e}^{-\beta H_\Xi}\, O_\Xi)$ where Tr stands for trace, $\beta = 1/kT$ where T is the temperature and O is a gauge invariant operator. This quantity is given explicitly by

$$\sum_{n,m} \langle n_\Xi|\exp(-\beta H_\Xi)|m_\Xi\rangle\, \langle m_\Xi|O_\Xi|n_\Xi\rangle.$$

If the states $|n_\Xi(t)\rangle$ over which the trace is taken are the exact solutions of the Hamiltonian [the solutions given in (9)] then using equations (13) and (15) this trace becomes

$$\mathrm{Tr}\, \mathrm{e}^{-\beta H_\Xi} O_\Xi = \mathrm{e}^{\beta e \partial\Xi/\partial t}\, \mathrm{Tr}\, \mathrm{e}^{-\beta H_0}\, O_0\,, \tag{20}$$

where the trace on the right is taken over states with $\Xi = 0$. If O is the unit operator we obtain a formally gauge (and time) dependent partition function $Z_\Xi(t) = \mathrm{e}^{\beta e \partial\Xi/\partial t} Z_0$, where $Z_0 = \mathrm{Tr}\, \mathrm{e}^{-\beta H_0}$. The free energy given by $F = -kT\ln(Z)$ is $F_\Xi = -kT\ln(Z_0) - \mathrm{e}\partial\Xi/\partial t$. It is gauge dependent, but its derivatives with respect to thermodynamic variables, which give observable thermodynamic quantities, do not contain Ξ and so are gauge independent. The statistical average of any gauge invariant operator $\langle O_\Xi\rangle = \mathrm{Tr}(\mathrm{e}^{-\beta H_\Xi} O_\Xi)/Z_\Xi$, for example a spatial correlation function, is gauge independent because the factors involving the gauge function in the numerator and denominator cancel. If the internal energy obtained from the statistical average of the Hamiltonian operator is calculated, it, like the free energy, has a gauge dependent part. However, differences of internal energy, like differences of free energy, are gauge independent. We conclude that all observable quantities calculated with statistical mechanics are independent of gauge.

6. Time-dependent Perturbations

When the perturbing fields and potentials depend on time, the wave equation will have the form of (16) with V being a small perturbation that is now time dependent. In this circumstance we express the wavefunction in the form

$$\Psi_\chi(\mathbf{r},\, t) = \sum_n a_n(t)\, \Psi_{\chi,n}(\mathbf{r},\, t)\,, \tag{21}$$

where the $\Psi_{\chi,n}(\mathbf{r},\, t)$ are the basis functions of (9) containing the $\psi_n(\mathbf{r})$ that are solutions of $H_0{}^0\, \psi_n(\mathbf{r}) = E_n\, \psi_n(\mathbf{r})$ given in (8) for the time-independent potentials $\mathbf{A}^0$ and ϕ^0 but now the a_n are time dependent. If the explicit form, given by (9), of the wavefunction of (21) is substituted into (16) then, with the help of the result

$$[H^0_\chi - \mathrm{i}\hbar\partial/\partial t]\Psi_\chi(\mathbf{r},\, t) = -\mathrm{i}\hbar \sum_n \psi_n(\mathbf{r}) \exp[\mathrm{i}(e\chi - E_n t)/\hbar]\; (\mathrm{d}a_n/\mathrm{d}t)\,, \tag{22}$$

and after using the relation $V_\chi = \exp(\mathrm{i}e\chi/\hbar)\, V_0 \exp(-\mathrm{i}e\chi/\hbar)$ and making the appropriate cancellations the gauge function disappears altogether and the result

$$\mathrm{i}\hbar \frac{\mathrm{d}a_m}{\mathrm{d}t} = \sum_n \mathrm{e}^{\mathrm{i}(E_m - E_n)t/\hbar}\, a_n\, V_{mn}(t) \tag{23}$$

is obtained where

$$V_{mn}(t) = \int \psi^*_m(\mathbf{r})\, V_0(t)\, \psi_n(\mathbf{r})\; \mathrm{d}\mathbf{r}\,. \tag{24}$$

Equations (23) and (24) are exactly the same as those obtained in the conventional treatment of quantum mechanics where the gauge function is set to zero throughout (Cohen-Tannoudij *et al.* 1977).

The probability amplitude in arbitrary gauge for the system to be in state m at time at t is defined to be $\int \Psi^*_{\chi,m}(\mathbf{r},\, t)\, \Psi_\chi(\mathbf{r},\, t)\, d\mathbf{r}$. By using equations (9) and (21) and the orthonormality of the $\psi_n(\mathbf{r})$ this amplitude is found to be simply $a_m(t)$. This also is identical to that obtained when $\chi = 0$. That this should be the case is not immediately obvious. The conventional procedure for carrying out a gauge invariant calculation, summarised in Section 1, is to start with a gauge invariant equation of motion, such as the Schrödinger equation, and then set the gauge function to zero. Although the results so obtained are valid for zero gauge explicitly they are known to be valid (in the sense that observable quantities produced by the calculation are independent of gauge) also for arbitrary gauge because the equation of motion is gauge invariant. On this basis a conceivable expression that *might* have been obtained for the probability amplitude with arbitrary gauge *might* have included some function of the gauge function itself, for example, $\exp(ie\chi/\hbar)a_m(t)$. The squared modulus of this would give the required gauge independent probability. If it were obtained with a conventional gauge invariant calculation that took $\chi = 0$, the probability amplitude would be just $a_m(t)$ and the gauge factor would not be visible. However, as shown in this section, this hypothetical possibility is not realised in practice. It has been found that the gauge-*explicit* probability amplitude is $a_m(t)$ which does not contain χ at all. Probability amplitudes are independent of gauge.

7. Comment

It is reasonable to ask what the point is of demonstrating in detail that the results of measuring physically observable quantities do not depend on gauge when it is known from the start that the quantum wave equations themselves are gauge covariant and that therefore all their physical consequences must be independent of gauge. An answer to this question is that, apart from the purely intellectual interest in seeing the details of how arbitrary gauge may be incorporated explicitly into quantum mechanics, a contribution has been made to resolving an issue which has caused controversy in the literature cited in this paper.

This issue concerns perturbation theory, the nature of the basis states between which transitions are caused by a perturbing field and the definition of the probability amplitudes relating to them. It has been found that because the gauge function is time dependent the time-dependent Schrödinger equation must be used *always* and that the basis states are therefore time dependent but can be defined for time-independent fields only, both for time-dependent and time-independent perturbations. The principle that physical quantities be gauge independent requires that probabilities be independent of gauge. However, it emerges in Section 6 that a stronger condition holds, namely that probability *amplitudes* are independent of gauge and are therefore identical to those used in the conventional version of quantum mechanics in which gauge is ignored.

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