Stokes-Einstein law. Keyes and Oppenheim[7] have presented a hydrodynamic bilinear mode-coupling derivation based on the Mori formalism which also leads to a factor of $\frac{1}{5}$. A hydrodynamic calculation using the Navier-Stokes equation with "stick" boundary condition ("slip" boundary condition) for the fluid velocity at the surface of the Brownian particle predicts $\frac{1}{6}$ ($\frac{1}{4}$). It is intriguing that kinetic theory, which requires no boundary condition, yields a factor intermediate between these hydrodynamic extremes.

The generalized repeated-ring kinetic theory yields the same asymptotic behavior as the ring kinetic theory since the latter already includes the most divergent contribution. However, D, which requires the full time behavior of $\psi_v^B(t)$, satisfies the Stokes-Einstein relation only for the generalized repeated-ring theory. This suggests that the theory used here should be investigated as a theory of equilibrium time correlation functions in dense fluids.

Finally, we emphasize that the kinetic equation used here, while physically plausible, has not been derived for a dense fluid. We are currently investigating its derivation.

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Hamiltonian Expectation Values for Time-Dependent Foldy-Wouthuysen Transformations: Implications for Electrodynamics and Resolution of the External-Field πN Ambiguity

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Although the time-dependent Foldy-Wouthuysen (FW) transformation of the "Schrödinger" equation $i\partial\psi/\partial t = H\psi$ yields the transformed equation $i\partial\psi'/\partial t = H'\psi'$, where $\psi' = U\psi$ and $H' = UHU^{-1} - iU\partial(U^{-1})/\partial t$, the expectation values $(\psi_1, H\psi_j)$ of H are not equal to $(\psi_i', H'\psi_j')$, but rather, to $(\psi_i', UHU^{-1}\psi_j')$. But one still has $(\psi_i', \psi_j') = (\psi_i, \psi_j)$. I discuss implications for perturbation calculations, scattering amplitudes, electrodynamics, and the external-field πN ambiguity, and look at exact special cases.

In their classic paper,[1] Foldy and Wouthuysen (FW) showed that a relativistic time-dependent "Schrödinger" equation

$$i(\partial/\partial t)\psi = H\psi, \tag{1}$$

after undergoing a time-dependent unitary transformation U, is given by the Schrödinger equation (dot signifies $\partial/\partial t$)

$$i(\partial/\partial t)\psi' = H'\psi', \quad \psi' = U\psi, \tag{2}$$

$$H' = UHU^{-1} - iU\dot{U}^{-1}. \tag{3}$$

More specifically, Foldy and Wouthuysen were interested in starting with the external-field Dirac electromagnetic Hamiltonian

$$H = \gamma_0\vec{\gamma}\cdot(\vec{p} - e\vec{A}) + \gamma_0 m + eV, \tag{4}$$

and then using successive transformations to diagonalize H order by order in $1/m$ (in the sense of decoupling the positive-energy components from the negative-energy components). FW found that by using Eq. (3) they could transform the Dirac Hamiltonian to order $1/m^2$ into the generalized Pauli time-dependent Hamiltonian[1]

$$H_P = \gamma_0\left(m + \frac{(\vec{p} - e\vec{A})^2}{2m}\right) + eV - \frac{e}{2m}\gamma_0\vec{\sigma}\cdot\vec{B} - \frac{ie}{8m^2}\vec{\sigma}\cdot(\nabla\times\vec{E}) - \frac{e}{4m^2}\vec{\sigma}\cdot(\vec{E}\times\vec{p}) - \frac{e}{8m^2}\nabla\cdot\vec{E}, \tag{5}$$

with

$$\vec{E} = -\nabla V - \dot{\vec{A}}, \quad \vec{B} = \nabla \times \vec{A}. \tag{6}$$

It has often been tacitly assumed, therefore, that the Pauli Hamiltonian is equivalent to the Dirac Hamiltonian, to this order. However, as I now observe, H' is *not* physically equivalent to H. This holds since, although

$$(\psi_i', \psi_j') = (\psi_i, U^{-1}U\psi_j) = (\psi_i, \psi_j), \tag{7}$$

(as in, for example, a discussion of the scattering amplitude from "in" and "out" states), the physical matrix elements of H and H' are *not* the same. In particular,

$$\begin{aligned}(\psi_i, H\psi_j) &= (\psi_i, (U^{-1}U)H(U^{-1}U)\psi_j) \\ &= (\psi_i', (UHU^{-1})\psi_j') \neq (\psi_i', H'\psi_j').\end{aligned} \tag{8}$$

Thus, although Foldy and Wouthuysen were correct in showing that it is H' which determines the time development of the transformed wave function, H' is not equivalent to H in the sense of having the same matrix elements. Rather, UHU^{-1} is. (In fact, any operator A would have its transformed matrix elements preserved by considering UAU^{-1}.)

Note that my observation is strikingly verified in the trivial special case where $H = H_0$, the free time-independent Hamiltonian, and $U = \exp(-i\omega t)$. Then $H' = UHU^{-1} + \omega$, so that $(\psi', H'\psi') = (E_0 + \omega)$, *not* E_0. Further, it has been pointed out to me that even in classical mechanics a time-dependent canonical transformation can cause an energy shift.[2] At its roots this problem focuses on the Hamiltonian formulation of mechanics with its special treatment of the time variable.

One may wonder, then, why standard calculations using H' (such as perturbation theory with the Pauli Hamiltonian) have yielded experimentally correct numbers. I give here two methods to see why, the first coming from a slightly involved and specialized perturbation-theory argument. If one can assume the Schrödinger statement that the *total* time derivative of the quantity $U^{-1}V_0$ defined below is zero; $[U^{-1}V_0, H] = -\dot{U}^{-1}V_0$; then one can arrive at

$$(\Psi_i, H\Psi_j) = (\Psi_{i0}', H'\Psi_{j0}'), \quad \Psi_{j0}' \equiv V_0\Psi_j, \tag{9}$$

where the Ψ are any wave functions (ψ_0, or something else, and not necessarily ψ), and V_0 is a time-*independent* unitary transformation. The difference between Ψ' and Ψ_0' can be mocked up by $-iU\dot{U}^{-1}$. Paradoxically, this implies it *can* be possible to get the same energy expectation values from a perturbation theory because one is *not* taking the exact expectation values of the transformed Hamiltonian. [Equation (8) shows that the exact expectation values would not be equal to the originals.] The second and more direct answer to the implied question is that as a matter of principle Eq. (7) shows that the exact scattering matrix obtained from the transformed wave functions *is* equal to the exact scattering matrix obtained from the original wave functions, even though in practice one cannot calculate such quantities. What is different about this situation from the time-independent case is that Eqs. (7) and (8) are not either both equalities or both inequalities.

I summarize the above paragraph: If one deals with time-dependent Hamiltonians and FW transformations in an external-field problem, the exact transformed wave functions ψ', whose time evolution is described by the transformed Hamiltonian H', would yield the same scattering amplitudes as in principle would be obtained from the original wave functions ψ of Eq. (1). However, H' *would not* yield the same energy expectation values as H. UHU^{-1} would, as I now elucidate.

Even though c-number, single-particle, relativistic wave equations have well-known difficulties when interactions are introduced, this all has interesting consequences if one chooses to discuss such an external-field problem. When one uses a particular external-field Hamiltonian in a Schrödinger equation, one is saying that this Hamiltonian—and this Hamiltonian alone (up to time-dependent transformations)—gives both the time development of the Schrödinger equation *and* the object to consider for *exact* physical matrix elements. An external-field single-particle Hamiltonian conceals the fact that physically it is the *total* coupled-field Hamiltonian which need be invariant. The coupled Hamiltonian only implies that the energy of the entire system is conserved under a time-dependent transformation, not necessarily a piece of it (the external-field problem).

This has escaped general notice for two reasons, both related to the Pauli Hamiltonian. We have seen that the Pauli Hamiltonian is equivalent to the nonrelativistic Dirac Hamiltonian in the static case ($\dot{A} = 0$, $\dot{U}^{-1} = 0$), like the hydrogen atom. Since it also turned out that perturbation calculations indicated equivalence, it has sometimes been assumed to be true exactly. The second reason is that with the $U\dot{U}^{-1}$ term, the Pauli Hamiltonian is written in terms of the gauge-invariant electric field $\vec{E} = -\nabla V - \dot{\vec{A}}$.[3] However, al-

though that is esthetically pleasing, it can be misleading.[4] For all theories it is necessary that the physical matrix elements remain the same.

My observations also allow us to solve the πN Galilean-invariant ambiguity. (One will also see that considering UHU^{-1} in the end will yield the correct static pion-field contribution to the nucleon mass.) For many years now[5-11] discussions have existed on how or even whether the relativistic πN Hamiltonian will lead to a nonrelativistic Galilean-invariant interaction. In particular, it has *not* been demonstrated that the exact, relativistic, *c-number* pseudoscalar πN Hamiltonian (which Hamiltonian can be considered a model for the nuclear force problem)

$$H=\gamma_0\vec{\gamma}\cdot\vec{\mathrm{p}}+\gamma_0 M+ig\varphi\gamma_0\gamma_5 \tag{10}$$

(φ being the pion field) must yield the Galilean-invariant nonrelativistic interaction

$$H_{\mathrm{nr}}=\frac{g}{2M}\left[\vec{\sigma}\cdot\nabla_\pi\varphi-\frac{m_\pi}{m_N}\varphi\vec{\sigma}\cdot\nabla_N\right]. \tag{11}$$

This problem was beautifully focused by Barnhill,[8] who in a set of detailed calculations considered the three unitary, time-dependent FW transformations $U_{a,b,c}$,

$$U_{a,b,c}{}^{\pm1}=\exp(\pm iS_{a,b,c}),\quad S_{ab}=\lambda S_{1,2}+(1-\lambda)S_{2,1}, \tag{12}$$

$$S_1=(g\varphi/2M)\gamma_5,\quad S_2=(-i/2M)\vec{\gamma}\cdot\vec{\mathrm{p}},$$
$$S_c=(ig\dot{\varphi}/4M^2)\gamma_0\gamma_5, \tag{13}$$

where $0\leq\lambda\leq1$. Barnhill demonstrated that if one successively applies these transformations to the Hamiltonian (10) in the stardard manner[1] of Eq. (3) for obtaining H', one finds to order M^{-2} and g that

$$H'=M\gamma_0+\left(\frac{\vec{p}^{\,2}}{2M}\right)\gamma_0+\frac{ig}{2M}\gamma_0\gamma_5\vec{\gamma}\cdot\vec{\mathrm{p}}_\pi\varphi$$
$$+\frac{g}{4M^2}\gamma_5\lambda(\vec{\gamma}\cdot\vec{\mathrm{p}}\dot{\varphi}+\dot{\varphi}\vec{\gamma}\cdot\vec{\mathrm{p}}). \tag{14}$$

For $\lambda=1$ the last two terms can be approximated[8] to the Galilean-invariant interaction, but for $\lambda\neq1$ this does not ensue. Thus, one seems to have an energy ambiguity in the Hamiltonian.[12]

Part of the resolution should now be clear. One should use UHU^{-1} instead of H'. If one does this, then the Barnhill transformations give only the first three terms of H' and there is no λ ambiguity. But where, then, is the Galilean invariance? That is hidden in the third term on the right-hand side which reduces to $(ig/2M)\vec{\sigma}\cdot\vec{\mathrm{p}}_\pi\varphi$ on the large components.

One must remember that this is an external-field problem which has dropped the second coupled field equation $(\Box+m_\pi^2)\varphi=-ig\bar{\psi}\gamma_5\psi\varphi$. Therefore, just as the hydrogen atom ignores the momenta of the proton with respect to the electron, so too this problem ignores the relative momenta of the pion with respect to the nucleon. It is a funny external-field problem since the nucleon is in the external field of the pion which is allowed to move. Thus, to go to center-of-mass coordinates one makes, on physical grounds, the substitution

$$\vec{\mathrm{p}}_\pi\rightarrow\vec{\mathrm{p}}_\pi-(m_\pi/m_N)\vec{\mathrm{p}}_N. \tag{15}$$

Note that I am not necessarily identifying M with m_π or m_N. M is the unusual reduced mass of the proton in the external field of the pion which is allowed momenta. But that is not the point. The point is that the c-number relativistic Hamiltonian reduces to an unambiguous Galilean-invariant interaction. However, for a complete understanding in the pion absorption case, it is clear that both coupled quantum field equations must be considered. That is, preferably one should perform a time-dependent FW transformation first, and then decouple the equations to the nonrelativistic limit.

To obtain a physical feeling for the correctness of this resolution, one can obtain and study the exact spectra of the Hamiltonian in the case where the pion field is only a function of time, $\varphi=\Phi(t)$. First, since $\vec{\mathrm{p}}$, M, and $\Phi(t)$ all commute, obtaining the spectra of H in Eq. (10) is simply finding the eigenvalues of a matrix. One finds that the spectra of H are

$$\pm\mathcal{E}(t)=\pm[M^2+p^2+g^2\Phi^2(t)]^{1/2}. \tag{16}$$

However, the spectra of H' from U_a are not $\pm\mathcal{E}(t)$, but $\pm[\mathcal{E}^2+\mathcal{D}\pm\Delta]^{1/2}$, where $\mathcal{D}$ and Δ are complicated functions of λ, $\vec{\mathrm{p}}$, Φ, and $\dot{\Phi}$. On the other hand, as one might expect for unitary transformations, the spectra of $U_aHU_a{}^{-1}$, $U_bU_aHU_a{}^{-1}U_b{}^{-1}$, and $U_cU_bU_aHU_a{}^{-1}U_b{}^{-1}U_c{}^{-1}$ are all $\pm\mathcal{E}(t)$. This can be shown exactly by using the mathematical methods described by Krajcik and Nieto[13,14] for writing a matrix functional $f(A)$ in closed form. In particular, these methods allow one to give the exact, closed forms of $U_{a,b,c}{}^{\pm1}$ when $\varphi=\Phi(t)$. Thus, the unitarily transformed Hamiltonians can be given in closed form so that the spectra can be calculated. Specifically, the exact trans-

formations are

$$U_{a,b}{}^{\pm 1} = (\cos K_{a,b})I \pm (i/K_{a,b})(\sin K_{a,b})S_{a,b}, \quad (17)$$

$$K_{a,b} = + \left[\left(\Lambda_{a,b} \frac{g}{2M} \right)^2 + (1 - \Lambda_{a,b})^2 \frac{p^2}{4M^2} \right]^{1/2}, \quad (18)$$

$$\Lambda_a = \lambda, \quad \Lambda_b = 1 - \lambda, \quad (19)$$

$$U_c{}^{\pm 1} = \left(\cos \frac{g\dot{\Phi}}{4M^2} \right) I \mp \left(\sin \frac{g\dot{\Phi}}{4M^2} \right) \gamma_0 \gamma_5. \quad (20)$$

Finally, one can find the FW transformation which exactly diagonalizes H of Eq. (10) when $\varphi = \Phi(t)$. Again by the methods of Refs. 13 and 14, with the aid of the standard free Lorentz transformation given on p. 30 of the second work in Ref. 1, this transformation is

$$U^{\pm 1} = [\, 2\mathcal{E}(\mathcal{E} + M)]^{-1/2} [(\mathcal{E} + M) I \pm \vec{p} \cdot \vec{\gamma} \pm ig\Phi\gamma_5], \quad (21)$$

which yields

$$UHU^{-1} = \mathcal{E}(t)\gamma_0. \quad (22)$$

Note that in the completely static case, where the pion field is a constant, Eq. (22) is the exact FW transformation which gives the energy eigenvalues. Hence this is another way to show that a constant, static pion field adds a term to the nucleon effective mass.

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