TDHF-LIKE EQUATIONS IN FIELD THEORY AND CONDENSED MATTER SYSTEMS

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"Es war getan, fast eh' gedacht."

Goethe

ABSTRACT

We discuss qualitatively a number of examples of TDHF-like equations that have arisen in model field theories and in (more physically relevant) quasi-one-dimensional condensed matter systems. These examples illustrate several phenomena seen in the (technically much more complicated) applications to nuclear physics and offer a new and perhaps invigorating perspective on TDHF.

I. INTRODUCTION

In this article, which is intended to provide a diversion from the focus of these proceedings on applications of TDHF to nuclear physics, I shall offer a very brief glimpse of some recent results (mostly not my own) on TDHF-like equations in field theory and condensed matter physics. Considerations of length have compelled me to select only three main topics -- the Gross-Neveu model,[1] a coupled electron-phonon model for the linear polymer polyacetylene $[(CH)_x]$,[2] and the ϕ^4 field theory coupled to fermions[3] -- and to treat even these limited topics sketchily. Hopefully, those intrigued by the results will pursue these subjects using the references in the incomplete but representative bibliography.

To anticipate here a question asked to me explicitly during the conference by Hubert Flocard, I should note that "the Fock is a fake", since none of the explicit calculations I describe includes exchange terms. In some cases -- for example for bound states in the Gross-Neveu model -- one can show that this absence of exchange terms is physically correct,[4] but in others -- scattering of the nonlinear excitations, for instance -- exchange terms should in general be included.

II. THE GROSS-NEVEU MODEL

The Gross-Neveu model,[1] a relativistic field theory in one space dimension and time, has proven to be one of the most productive theoretical laboratories of recent years. The Lagrangian density of the theory can be written in the (suggestive) form (see references 1 and 4 for details of notation)

$$(x,t) = \sum_{\alpha} \bar{\psi}^{(\alpha)}(x,t)\ (i\gamma^{\mu}\ \partial_{\mu} - g\sigma(x,t))\ \psi^{(\alpha)}(x,t) - \frac{1}{2}\ \sigma^2(x,t) \qquad (1)$$

Here $\mu = (0,1)$ for time and space, respectively, $\psi^{+} = (u^{+}d^{+})$ is a two component Dirac field,[5] and $\alpha = 1, 2, \cdots N$ is an internal symmetry index corresponding to different "types" of fermions. As Hagen Kleinert mentioned in his contribution to the conference, the large N limit offers some simplifications and has been studied extensively.[1,6] The formal field equations which follow by varying the action corresponding to (1) are

$$\left\{ i\gamma_o \frac{\partial}{\partial t} + i\ \gamma_1 \frac{\partial}{\partial x} - g\sigma(x,t) \right\} \psi(x,t) = 0 \qquad (2.a)$$

and

$$g\sigma(x,t) = -g^2\ "\bar{\psi}\psi"\ . \qquad (2.b)$$

Assuming that the formal expression "$\bar{\psi}\psi$" does not hide too many pathologies, these equations are clearly of the form of (a relativistic generalization of) the familiar TDHF equations, with a "self-consistent" mean field (σ) determined by the fermion field (ψ). In fact, Dashen, Hasslacher, and Neveu[4] have shown, using the stationary phase approximation to a functional integral (cf. John Negele's contribution to these proceedings), that equations (2) are the semi-classical approximation to the quantum field theory and that the solutions to (2) do give the bound states (i.e., the particle spectrum) of the quantum theory provided that (1) $\sigma(x,t)$ is a periodic function of time and (2) $\psi(x,t)$ is a set of wavefunctions, anti-periodic in time. The formal expression "$\bar{\psi}\psi$" becomes the sum over all "occupied" wave functions. If, for definiteness, we seek solutions for which $\sigma(x,t)$ is static (a special case of periodic), the occupied states become just the negative energy "Dirac sea" plus, for calculation of the mass spectrum, a single positive energy state (ψ_o) with occupation number $1 \leq n_o < N$. Thus, Eq. (2.b) becomes

$$Z(\Lambda)\ g\sigma = -g^2 "\bar{\psi}\psi" = -g^2 \sum_{\text{occ.},\alpha} \bar{\psi}^{(\alpha)}\psi^{(\alpha)}$$

$$= -g^2\ n_o\ \bar{\psi}_o\psi_o - g^2 \sum_{\varepsilon<0,\alpha} \bar{\psi}^{(\alpha)}\psi^{(\alpha)} \qquad (2.b')$$

Here $Z(\Lambda)$ is the (infinite as $\Lambda \to \infty$) renormalization required to make (2.b′) sensible when the momentum cut off $\Lambda \to \infty$ (in which limit there are an infinite number of states in the sum over occupied levels). I mention this technical point primarily to indicate a subtlety that besets any attempt to extend TDHF formalisms to include

the "negative energy sea" of a relativistic theory. The generalization of (2.b´) for time periodic σ has the same structure,[4] except that the "energy" is replaced by the "Floquet index". For both the static and time-periodic cases, soliton-like solutions to Eqs. (2) are known and have been used to calculate the particle spectrum of the theory. Interestingly, one class of soliton solutions[4] ("bags" and "breathers") leads to a sequence of particles (the analogs of "nuclei") with 1, 2, ··· 3 (<N) fundamental constituents ("nucleons") as well as particles corresponding to the σ field ("mesons") and particles made of "nucleons", and "mesons" (the analogs of the "Δ" and other "isobars"). Amusingly, a second class of soliton solutions[4] (the "kinks") leads to one-dimensional analogs of Lee-Wick "density isomers" or "abnormal nuclei",[7] which are very massive in the large N limit. These results on bound states (at least for the "normal nuclei") are directly analogous to TDHF calculations of large amplitude collective oscillations[8] of a range of different nuclei. For application to the scattering of two "nuclei", which has not been studied in the Gross-Neveu model, the boundary conditions on and/or the form of the Eqs. (2) would be expected to change, along the lines suggested in Hugo Reinhardt's contribution to these proceedings.

One reason that scattering in the semi-classical approximation has not been investigated is that there exists an exact, analytic expression for the S-matrix of the full quantum field theory.[9,10] Thus one has the ideal case in which, as stressed here by John Negele, non-trivial tests of the semi-classical approximations can be made. For the bound states one finds that the spectrum of the full quantum theory is the same as that calculated semi-classically,[4] provided one replaces N by N-1.[9,10] Thus, as anticipated, for $N \to \infty$ the semi-classical limit is valid.

The analytic accessibility of the exact quantum S-matrix is a consequence of the complete integrability[9-12] of the Gross-Neveu model. This is a very special feature, and thus it is useful to note that apart from this exact analytic comparison, one can use recent (and more generally applicable) Monte Carlo calculations of the full quantum theory as tests of the TDHF-like approximations; this work is currently in progress.[13]

Finally, from the TDHF perspective a perhaps unfamiliar aspect of Eqs. (2) is the relativistic kinematics. It is thus interesting to observe that, for weakly bound "nuclei" -- here this is equivalent to the requirement $n_o/N \ll 1$ -- there is a well-defined non-relativistic reduction of Eqs. (2).[14] Introducing $V(x) \equiv g\sigma(x)-m$ and keeping only the u component of the wave function ψ_o -- the d component is O(1/m) in this limit -- one finds

$$i \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} - V(x,t)\, u \cong 0 \qquad (3a)$$

and

$$V(x,t) \cong -g^2 n_o |u|^2 , \qquad (3b)$$

which combine to yield precisely the famous nonlinear Schrödinger equation, familiar as the TDHF approximation to the one-dimensional δ-function potential system.

III. THE ELECTRON-PHONON MODEL OF TRANS-POLYACETYLENE ($(CH)_x$)

It is hopeless, given length constraints, for me to provide the full appropriate background for the following discussion of the coupled electron-phonon model[2] of trans-polyacetylene ($(CH)_x$); interested readers are referred to the literature.[15] To make the mathematical symbols clear, however, I must note that trans-$(CH)_x$ is a (quasi-) one dimensional (infinite, for theorists) polymeric chain consisting of (CH) units connected, in the ground state configuration, by alternating double bonds, as is shown in the chemical diagrams of Figs. 1b and 1c.

The kinematics of the microscopic electron-phonon model of $(CH)_x$ can be seen from Fig. 1a. Two of the three bonds available for each (CH) unit are treated as given and non-dynamic, and the problem of modelling the system is reduced to describing the coupled motion of the backbone "lattice" of (CH) units -- u_n will indicate the displacement of the $n^{\underline{th}}$ (CH) unit from its equilibrium position -- and the one remaining electron per site ($c_n^+(c_n)$ will indicate the operator creating (annihilating) an electron at the $n^{\underline{th}}$ site). Actually c_n^+ and c_n should also have a spin

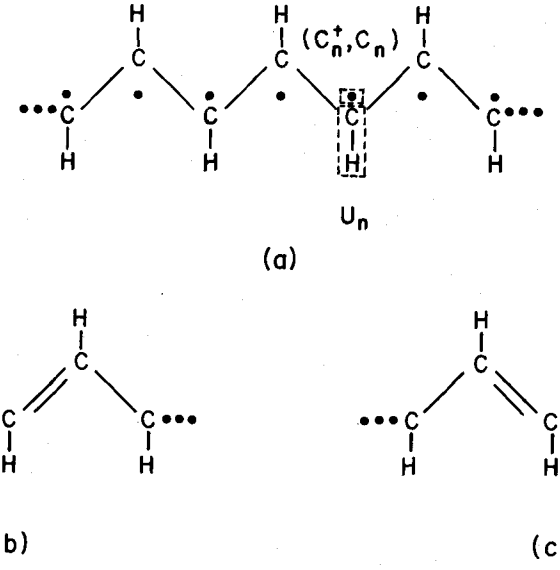

Fig. 1. (a) A sketch indicating the relation of dynamical variables (u_n, and (c_n^+,c_n)) to the chemistry of trans-$(CH)_x$; (b) and (c) short segments of the chemical structures corresponding to the two degenerate ground states of trans-$(CH)_x$.

label, s, corresponding to the two spin states of the electron. For simplicity, I will suppress this here.

The lattice Hamiltonian[2] describing $(CH)_x$ has the form

$$H = \frac{M}{2} \Sigma \left(\frac{\partial u_n}{\partial t}\right)^2 + \frac{K}{2} \Sigma (u_{n-1}-u_n)^2$$

$$- \Sigma t_o (c^+_{n-1} c_n + c^+_n c_{n-1}) \qquad (4)$$

$$- \Sigma \alpha(u_{n-1}-u_n)(c^+_{n-1} c_n + c^+_n c_{n-1}) ,$$

Here the four terms represent respectively (1) the kinetic energy of the lattice, (2) the bond strain energy caused by lengthening or shortening distances between adjacent units, (3) the constant "hopping" of an electron from one site to the next and (4) the coupling of the lattice and electron motions. For <u>trans</u>- $(CH)_x$ the Hamiltonian in Eq. (4) must be supplemented by the requirement that precisely one half of the electron states - starting from the lowest state - are filled. From the equations of motion corresponding to (4) one can show analytically that the ground state is two-fold degenerate, as in Figs. 1b and 1c. To go much beyond this requires numerical studies,[2,16] and rather than pursue those results, I shall consider the continuum limit[17-20] -- the lattice spacing $a \to 0$ -- of H, in which analytic progress can be made. This has the dual advantages that the TDHF-like nature of the polyacetylene equations is obvious and further that an amusing connection[21,22] between polyacetylene and the Gross-Neveu model becomes evident. In the continuum limit, the Hamiltonian in (4) becomes[17-20]

$$H_c = \int dx \left\{ \frac{M}{2}\left(\frac{\partial \Delta(x,t)}{\partial t}\right)^2 + \frac{1}{2}\frac{\omega_Q^2}{g^2} \Delta^2(x,t) \right. \qquad (5)$$

$$\left. + \psi(x,t)^+ [-iv_F \sigma_3 \frac{\partial}{\partial x} + \sigma_1 \Delta(x,t)]\psi(x,t) \right\}$$

where $\Delta(x,t)$ is the (gap) parameter representing the lattice motion, σ_i is the $i^{\underline{th}}$ Pauli matrix, and $\psi^+ = (u^+ v^+)$ is a two component field[5] describing the electrons. The linear, Dirac-like kinetic energy for the electron is a result of expanding the lattice dispersion relation around the half-filled band and keeping only the leading term as $a \to 0$. Clearly, the general structure of this Hamiltonian is qualitatively like the energy functionals considered in TDHF. Specifically, the fermions (ψ) interact only via a mean field (Δ). Important <u>differences</u> from ordinary TDHF are (1) the requirement of filling the lowest one-half electron states -- the "negative

energy sea" in the pseudo-relativistic analog or the "valence band" in solid state terminology -- and (2) the presence in the Hamiltonian of time-dependence ($\equiv \dot{\Delta}^2$) for the mean field. Sadly, the presence of the $\dot{\Delta}^2$ term has prevented analytic solutions of the equations of motion corresponding to H_c except in the case of static mean fields, i.e., $\dot{\Delta} = 0$. Of course numerical studies can be carried out either on the semi-classical, mean field equations (by equation of motion methods[16] like TDHF) or on the full quantum theory (by Monte Carlo methods)[23] and comparison of the approximate and exact solutions is of great current interest. Here, I will focus on static Δ, in which case the equations of motion become[17-20]

$$\varepsilon_n \psi_n = -iv_F \sigma_3 \frac{\partial}{\partial x} \psi_n + \Delta \sigma_1 \psi_n \tag{6.a}$$

and

$$\Delta = \sum_{\varepsilon_n<0}{}' \psi_n^+ \sigma_1 \psi_n \ , \tag{6.b}$$

where in both equations the spin index ($s = \pm 1/2$) on the fermion wave function ψ_n has been suppressed. Once more the TDHF-like -- here again, really only Hartree-like -- nature of the equations is evident. The summation in (6.b) runs, for the ground state, over all states in the valence band -- which, because of the linear kinetic energy in (6.a) must be cut off by hand at an energy corresponding to the full band width -- plus, for excitations, any additional occupied states. The structure of Eqs. (6) is clearly very similar to that of the static Gross-Neveu model Eqs. [(2)] -- with $N = 2$ to correspond to the two spin degrees of freedom -- and in fact one can show that, at this static, mean field level, the equations are identical.[21,22] The solutions corresponding to nonlinear excitations must therefore also be the same. Indeed, the "kinks" of the Gross-Neveu model are in $(CH)_x$ the "kink" solitons with the celebrated exotic spin-charge relations.[2,18,24] The "bag" solutions of the Gross-Neveu model become "polaron" solutions -- since $N = 2$ there is only one (electron) polaron state ($n_o = 1$) -- which, although more conventional than kinks, are also more generic in the sense that they are expected to occur in a much wider class of quasi-one-dimensional polymers.[21,22] Even the analog of the non-relativistic reduction of the Gross-Neveu model is of interest; here, this corresponds to reducing[14] the polaron of Eqs. (6) to the more conventional polaron,[25] satisfying the nonlinear Schrödinger equation, familiar in solid state physics.

Since we have stressed the similar structure of the electron-phonon model of $(CH)_x$ and the $N = 2$ Gross-Neveu model, it is crucial to note the manifest difference: namely, the $\dot{\Delta}^2$ term in (5), which has no counterpart in (1). This term leads to important differences in the time-dependent and fully quantum versions of these models.

Finally, in $(CH)_x$ there is an important open question directly analogous to the questions of "residual interactions" and "collision terms" in applications of TDHF to nuclear physics. Specifically, the Hamiltonians in (4) and (5) include only electron-phonon coupling and involve no direct electron-electron coupling. At least the Coulomb part of this coupling -- which would, loosely speaking, be of the form $(\psi^+\psi)^2$ -- is expected to be important, and it is an unsolved problem to include these terms correctly and non-perturbatively. Monte Carlo methods can, of course be used, but some clever, at least partially analytic, extended mean field theory is clearly desirable.

IV. $\lambda\phi^4$ FIELD THEORY WITH FERMIONS

Our last example of TDHF-like equations in field theory is the one space dimensional $\lambda\phi^4$ theory coupled to fermions.[3] The Lagrangian density is

$$\mathcal{L}(x,t) = \frac{1}{2}\left(\frac{\partial\phi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 - \frac{\lambda}{4}(\phi^2-1)^2 + \sum_{\alpha=1}^{N} \bar{\psi}^{(\alpha)}\,(i\gamma\partial - g\phi)\psi^{(\alpha)} \tag{7}$$

The fermion term of the Lagrangian, including the linear coupling to the boson field ϕ, is clearly identical to that of the Gross-Neveu model. The purely bosonic part of has been used to describe the displacive limit of structural phase transitions in uniaxial ferroelectrics,[26] as a mean field theory of phase transitions involving one component order parameters ("Landau-Ginzburg theory"), and as a phenomenological -- as opposed to the previously discussed microscopic -- model of nonlinear excitations in polyacetylene.[27] The full Lagrangian has been studied, in the semi-classical approximation, as a "toy" model of nuclear physics in one dimension.[3,28] More specifically, the static field equations following from (7),

$$-\frac{\partial^2\phi}{\partial x^2} - \lambda\phi + \lambda\phi^3 = -g''\bar{\psi}\psi'' \tag{8.a}$$

and

$$(i\gamma_1\,\partial_x - g\phi)\psi_i = \gamma_o\,\varepsilon_i\,\psi_i\ , \tag{8.b}$$

have been solved analytically[3] using the same methods applied to the Gross-Neveu model. Again, both sequences of "normal nuclei" and "kinks" ("abnormal nuclei") are found as bound states. Of interest here from the TDHF perspective are the nonlinear interactions ($\lambda\phi^3$) and propagation effects ($\partial^2\phi/\partial x^2$) in the "mean" field. Once

again the full semi-classical approximation requires the inclusion of the infinite (for $\Lambda \to \infty$) negative energy sea. As sketched in the discussion of the non-relativistic reduction of the Gross-Neveu model, for weakly bound "nuclei", one can motivate a further approximation, in which only the single positive energy bound state (called ψ_0 previously) is kept in sum on the right-hand side of (8.a). Within this approximation -- which for definiteness we shall call the "Hartree approximation" -- two investigations closely parallelling familiar TDHF studies have been carried out. First, the fission decay of a large "nucleus" into two smaller "nuclei" has been calculated[29] using collective coordinate techniques for determining a "most probable" path in field space; this scheme is closely related to the adiabatic TDHF approach discussed in many contributions to these proceedings. Second, within the Hartree approximation, the time-dependent versions of Eqs. (8) have been used (without further justification) to study the scattering of two initially widely separated "nuclei".[30] The numerical results have shown the analog of the well-known "transparency"[8] of nuclear scattering in the TDHF approximation and, not surprisingly in view of our previous remarks, reduce to the analytically known results for the nonlinear Schrödinger equation for low relative velocities.

I will close with two comments on features found in the purely bosonic part of the Lagrangian in (8). Even in the absence of fermions, "kink" solitary wave solutions exist for the nonlinear equations for the field $\phi(x,t)$. The scattering of these kink solutions (actually, kink-antikink scattering) has been the subject of extensive study,[31-38] particularly because of an interesting sequence of resonances at low relative collision velocities. These resonances, for which a semi-phenomenological theory has recently been developed,[39] are the direct analogs of the fusion resonances seen at low collision velocities in one of the pioneering TDHF studies[8] of nuclear collisions. Finally, the use of the ϕ^4 theory (without fermions) as a phenomenological model -- with the field ϕ representing a bond length distortion -- of trans-$(CH)_x$[27] is an (indirect) example of the effective action approach suggested by Hagen Kleinert in these proceedings. In essence, the $(\phi^2-1)^2$ potential provides an approximate effective action that takes account of the effects of the electrons in the filled valence band in polyacetylene.[22]

I have presented a very brief "discussion" -- the term "index" may be more appropriate -- of a number of areas in field theory in which equations and/or results reminiscent of TDHF have arisen. Hopefully, the possibility of applications to a broader range of problems will stimulate further development of the concepts and methods of this interesting approach to quantum many body problems.

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