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Функциональный подход к самосогласованной теории, зависящей от времени

В рамках функционального подхода формулируется приближение теории Хартри-Фока, зависящее от времени.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Reinhardt H.

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Part Integral Approach to Time-Dependent Self-Consistent Field Theories

Toward a field theory of large amplitude collective motion we formulate the time-dependent Hartree approximation within a path integral approach.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

Recently path integral methods have been applied to the study of the nuclear many-body problem, mainly in connection with the foundation of the nuclear field theory [1,2,3]. Using path integral techniques we could give a complete derivation of the nuclear field theory [3]. In general, path integrals are a very convenient tool for deriving mean-field parturbation theories which are based on a small amplitude expansion (see, e.g., ref. [4].).

In the last years there is an increasing interest in the study of large amplitude collective motion, i.e., of such situations where a small amplitude expansion becomes meaningless (e.g., in strongly anharmonic systems). Most of these investigations have been performed in the framework of the time-dependent Hartree-Fock (TDHF) approximation (see, e.g., ref. [5]). It is interesting to see whether the TDHF theory can also be formulated within a path integral approach. A path integral formulation of the TDHF approximation could be advantageous in two respects: firstly, the path integral, which represents a link between classical and quantum mechanics, may prove useful in the quantization of (classical) periodic solutions to the TDHF equations. Secondly, it would allow one to calculate corrections to the quantized TDHF solutions in a systematic way. Therefore the present paper is devoted to a path integral formulation of the TDHF theory.

In the path integral approach to collective phenomena (called hereafter functional approach) the original fermion theory is replaced by an equivalent theory in a collective Bose field (see refs. [1,2,3]). Recently it has been shown for the Lipkin model that the (time-dependent) equation of motion of the corresponding collective field coincides up to some exchange terms with the TDHF equation [6,7]. In the present note we show for a general two-body interaction that, with a suitable choice of the collective field, the classical equation of motion of the collective field coincides with the time-dependent Hartree (TDH) equation. We restrict here the consideration, for simplicity, to the TDH equation, as the exchange terms do not appear in the functional approach on the same footing as the direct terms.

In the following we show how the TDH equation arises in the functional approach as a classical field equation.

The Lagrangian of an interacting Fermi system can be written as

$$\mathcal{L}(t) = \sum_{\alpha\gamma} a^{+}_{\alpha}(t)(i\partial_t \delta_{\alpha\gamma} - e_{\alpha\gamma})\, a_{\gamma}(t) - \frac{1}{2}\sum_{\alpha\beta\gamma\delta} a^{+}_{\alpha}(t)\, a_{\gamma}(t)\, V_{\alpha\gamma,\beta\delta}\, a^{+}_{\beta}(t)\, a_{\delta}(t)\,, \tag{1}$$

where $a^{+}_{\alpha}(a_{\alpha})$ are the fermion creation (annihilation) operators, $e_{\alpha\gamma}$ denotes the matrix elements of a one-body operator and $V_{\alpha\gamma,\beta\delta} = \langle\alpha\beta|V|\gamma\delta\rangle$ is the matrix element of the two-body interaction V. The generating functional for the fermion Green functions is given by the following path integral

$$Z[\eta,\eta^{+}] = N\int Da\,Da^{+} \exp[\,i\int dt(\mathcal{L}(t) + \sum_{\alpha}[\,a^{+}_{\alpha}(t)\,\eta_{\alpha}(t) + \eta^{+}_{\alpha}(t)\,a_{\alpha}(t)])\,]\,, \tag{2}$$

where the fermion operators are considered anti-commuting (Grassman) variables. Our aim is to transform the fermion theory defined by the Lagrangian (1) into an equivalent theory in a collective field. For this purpose we linearize the two-body interaction by means of a Bose field ρ so that the integration over the fermion variables a, a^+ can be carried out. Using the functional identity

$$\exp[-\frac{i}{2}\sum_{\alpha\beta\gamma\delta} a^+_\alpha a_\gamma V_{\alpha\gamma,\beta\delta}\, a^+_\beta a_\delta] = (\det V)^{1/2} \times$$

$$\times \int D\rho \exp[i\frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\rho_{\gamma\alpha} V_{\alpha\gamma,\beta\delta}\rho_{\delta\beta} + 2a^+_\alpha a_\gamma V_{\alpha\gamma,\beta\delta}\, \rho_{\delta\beta})]$$

we rewrite the generating functional (2) as

$$Z[\eta,\eta^+] = \int Da\, Da^+ D\rho \exp[i\int dt(\mathfrak{L}_c(t) + \sum_\alpha (a^+_\alpha \eta_\alpha + \eta^+_\alpha a_\alpha))] \qquad (3)$$

(the normalization constant is suppressed in the following) with the new effective Lagrangian

$$\mathfrak{L}_c(t) = \sum_{\alpha\gamma} a^+_\alpha(t)[i\partial_t \delta_{\alpha\gamma} - (e_{\alpha\gamma} + \sum_{\beta\delta} V_{\alpha\gamma,\beta\delta}\rho_{\delta\beta})]a_\gamma(t) + $$
$$+\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\rho_{\gamma\alpha}(t)V_{\alpha\gamma,\beta\delta}\,\rho_{\delta\beta}(t). \qquad (4)$$

Although the collective field appears in the functional integral (3) as an independent integration variable, it is indeed a composite field. Variation of the action $S_c = \int \mathfrak{L}_c(t)\,dt$ reveals its fermion structure

$$\rho_{\alpha\beta}(t) = a^+_\beta(t)\, a_\alpha(t). \qquad (5)$$

Defining the single particle Green function in the "external" field ρ via

$$G^{-1}_{\alpha\gamma}[\rho](t,t') = [i\partial_t \delta_{\alpha\gamma} - (e_{\alpha\gamma} + \sum_{\beta\delta} V_{\alpha\gamma,\beta\delta}\,\rho_{\delta\beta})]\delta(t,t') \qquad (6)$$

integration over the fermion variables in eq. (3) yields

$$Z[\eta,\eta^{+}] = \int D\rho \exp[\, iS[\rho] - i\int \sum_{\alpha\gamma} \eta^{+}_{\alpha}(t)\, G_{\alpha\gamma}(tt')\, \eta_{\gamma}(t')\, dt\, dt'] \qquad (7)$$

with the collective action $S[\rho]$ given by

$$S[\rho] = \int dt \Big(\frac{1}{2}\sum_{\alpha\beta\gamma\delta} \rho_{\gamma\alpha}(t)\, V_{\alpha\gamma,\beta\delta}\, \rho_{\delta\beta}(t) - i\,tr(\log G^{-1}[\rho])(t,t')\,\Big|_{t=t'-0}\Big), \qquad (8)$$

where the limit $t \to t'$ has been taken in accordance with the current $a^{+}a$ to which ρ couples in the Lagrangian (4). At the stationary points of the collective action defined by $\delta S/\delta\rho = 0$ the collective field takes the value

$$\rho_{\alpha\beta}(t) = -iG_{\alpha\beta}[\rho](t,t')\,\Big|_{t=t'-0}\,. \qquad (9)$$

Recalling the definition of the single particle Green function (in the Heisenberg picture)

$$G_{\alpha\beta}(t,t') = -i < T(a_{\alpha}(t)\, a^{+}_{\beta}(t')) > \qquad (10)$$

we obtain from eq. (9)

$$\rho_{\alpha\beta}(t) = < a^{+}_{\beta}(t)\, a_{\alpha}(t) >. \qquad (11)$$

Thus at the stationary points the collective field ρ coincides with the usual density matrix /8/. This result is in agreement with eq. (5).

The single particle Green function $G[\rho]$ defined via its inverse by eq. (6) has to satisfy the following equations

$$\sum_{\gamma} \int G^{-1}_{\alpha\gamma}[\rho](t,t'')\, G_{\gamma\beta}[\rho](t'',t')\, dt'' = \delta_{\alpha\beta}\,\delta(t,t'),$$

$$\sum_{\gamma} \int G_{\alpha\gamma}[\rho](t,t'')\, G^{-1}_{\gamma\alpha}[\rho](t'',t')\, dt'' = \delta_{\alpha\beta}\,\delta(t,t'). \qquad (12)$$

These equations together with eq. (9) constitute the equation of motion for the collective field ρ.

Using the definition of $G^{-1}[\rho]$, eq. (6), the last equations can be written as

$$\sum_{\gamma}[i\partial_t \delta_{\alpha\gamma} - h_{\alpha\gamma}]G_{\gamma\beta}(t,t') = \delta_{\alpha\beta}\delta(t,t')$$

$$\sum_{\gamma} G_{\alpha\gamma}(t,t')[i\partial_{t'}\delta_{\gamma\beta} - h_{\gamma\beta}(t)] = \delta_{\alpha\beta}\delta(t,t'), \tag{13}$$

where by comparison with eq. (11)

$$h^{(t)}_{\alpha\gamma} = e_{\alpha\gamma} + \sum_{\beta\delta} V_{\alpha\gamma,\beta\delta}\,\rho_{\delta\beta}(t) \tag{14}$$

is recognized as the standard Hartree-Hamiltonian (see, e.g., ref. /8/). Subtracting the second equation of eqs. (13) from the first one and taking the limit $t' \to t$ as defined in eq. (9) we obtain

$$i\partial_t \rho_{\alpha\beta}(t) = \sum_{\gamma}(h_{\alpha\gamma}\rho_{\gamma\beta} - \rho_{\alpha\gamma}h_{\gamma\beta}). \tag{15}$$

This is the familiar TDH equation for the density matrix.

We hope that the path integral formulation of the TDHF theory may be useful for quantizing the classical TDHF solution. To be more specific, in the path integral formulation the quantization could be performed in the semi-classical approximation as given by the field theoretic generalization of the WKB method developed by Dashen et al. /9/. The feasibility of such a "field theory" of large amplitude collective motion has been recently demonstrated for a schematic model /10/.

A more detailed discussion of a field theory of large amplitude collective motion will be presented elsewhere.

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