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原子・分子の相対論的高次相関計算アルゴリズム

Atomic Schwinger-Dyson Formalism, (Non-Perturbation Relativistic Field Theory for Atom and Molecules)

（Nano-Future Inc. Technova Inc. 東大先端研）松浦弘幸*
（産業医大情報）中野正博，（都立品川高専）根本哲也

1. Introduction

We propose Atomic Schwinger-Dyson formalism(ASD method) and renormalization under an external field in this paper, which is the nonperturbative and finite relativistic quantum field theory for a finite baryon and electron density. ASD can be applied to many of electron systems and electron matters. ASD consists of coupled Dyson equations of electrons and photons. It is shown that an electromagnetic field of ASD is separated into two parts, which are a mean field (classical field) and a fluctuation (quantum field). Because it includes self-energies in nonerturbative way, higher-order correlations beyond Hartee-Fock approximation are taken into account.

2. Schwiner-Dyson Method

In order to prepare for numerical calculations, we give a new explicit expressions of photon self-energies and electron self-energy, which are introduced for photons and electrons based on the particle-hole-antiparticle representation (PHA) of Atomic Schwinger-Dyson formalism (ASD). The PHA representation describes exactly the physical processes such as particle-hole excitations (electron-hole) and particle-antiparticle excitations (electron-positron). The self-energy of the electron includes both the quantum component and the classical component (classical external field and Coulomb's field) , which are divided into the scalar part of electron self-energy and 4-dimensional vector parts of the electron self-energy. The electron propagators are composed of the particle part, hole part and antiparticle part in PHA representation. The general representation of photon self-energy with 16 elements is expressed in terms of only two components, which are the transverse and longitudinal elements. The general form of the photon propagators are written in terms of free propagator for photon and two independent propagators (the transverse and longitudinal elements), which include two independent photon self-energies. The tensor part of the electron self-energy does not appear in ASD formalism which makes perfectly the closed self-consistent system, if we take the bare vertex approximation, $\Gamma^{\alpha}(p,q) \to \gamma^{\alpha}$.

Some important differences between the ASD formalism for the system of finite electron density and SD formalism of zero electron density are shown. The main difference is due to the existence of condensed photon field, what we call, Coulomb's potential and delayed potential. By paying special attention to the treatment of the condensed photon fields, the coupled Dyson equations of electron and photon are derived based on a functional propagator method. It is shown that this treatment of the condensed fields naturally leads to tadopole energy, which cancels Hartree energy. By using the photon propagator, explicit expression of ASD coupled equations and the energy density of matters are derived for numerical calculations. Similarities and difference between ASD and traditional methods such as the mean field theory or Hartree-Fock are discussed, it is shown that these traditional method are included in our ASD formalism.

In all quantum calculations, higher-order contributions from loop diagrams include an ultraviolet divergence. The real value of physical mass, electric charge and wave function are completely different from those of the non-renormalized electron and photon in

*pensukepen@ybb.ne.jp

mean field theory, since there are many of the particle-antiparticle creations and annihilations, particle-hole excitation, and Pauli blocking, and they give an effect on bare mass, electric charge, polarization of vacuum, and self-energy. ASD belongs to a well-defined class of field theories if this divergence could be removed systematically. We show that ASD method is renormalizable theory after small number of physical parameters are fixed from experiment.

Formalism and Explicit Expression

The starting point of our non-perturbation way is simple QED lagrangian density.

$$L = \bar{\psi}^e \left(i\gamma^\mu \partial_\mu - m\right)\psi^e + \bar{\psi}^p \left(i\gamma^\mu \partial_\mu - m\right)\psi^p$$
$$-\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{2}\varsigma\left(\partial_\sigma A^\sigma\right)^2$$
$$-e\bar{\psi}^e\gamma^\mu\psi^e A_\mu - e_p\bar{\psi}^p\gamma^\mu\psi^p A_\mu$$

The following equations of motions for the fields are derived from the generalized Euler-Lagrange equations: for electrons, nucleons, and photons:

$$\left(i\gamma^\mu \partial_\mu - m\right)\psi^e = e\gamma_\mu \psi^e A^\mu$$
$$\left(i\gamma^\mu \partial_\mu - M\right)\psi^p = e\gamma_\mu \psi^p A^\mu$$
$$\Box A^\mu - (1-\varsigma)\partial^\mu(\partial_\alpha A^\alpha) = e\bar{\psi}^e\gamma^\mu\psi^e + e_p\bar{\psi}^p\gamma^\mu\psi^p$$

Next step is to obtain the exact formal solutions of coupled Schwinger-Dyson equations, which are generated S-matrix with functional derivatives:

$$S = T\left[\exp\left\{i\int d^4x \cdot \left(e\bar{\psi}\gamma^\mu\psi A_\mu + \eta\bar{\psi} + \bar{\eta}\psi + J^\mu A_\mu\right)\right\}\right]$$

Finally, we reach the several explicit solutions with bare vertex approximation:

Particle-hole part of photon self-energy

$$\Pi^l_{hp} = \frac{-e^2 k^2_{(4)}}{(2\pi)^2 k^2}\int_0^{k_F}\int_{-1}^{1}\frac{n_p(1-n_Q)(2E_p^2 + E_p k_0 + pk\chi)}{E_p E_Q(E_Q - E_p - k_0)}p^2 dp d\chi$$

$$\Pi^t_{hp} = \frac{e^2}{(2\pi)^2}\int_0^{k_F}\int_{-1}^{1}\frac{n_p(1-n_Q)(E_p k_0 - pk\chi)}{E_p E_Q(E_Q - E_p - k_0)}p^2 dp d\chi$$

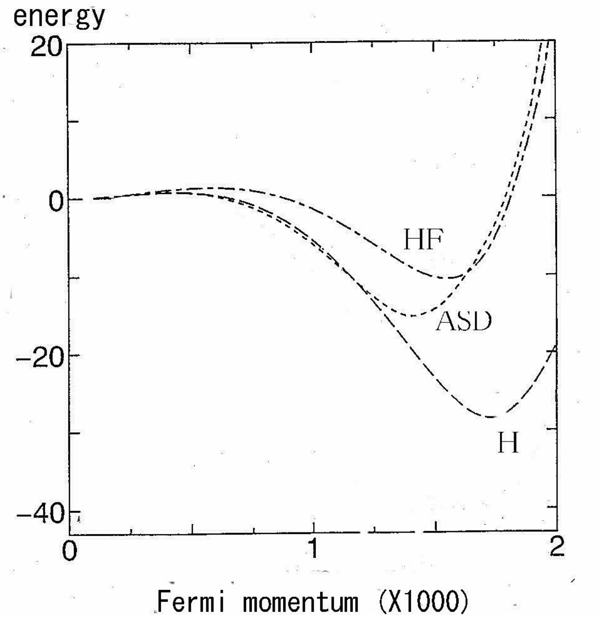

Fig.1 ASD, Harterr and Hartree-Fock

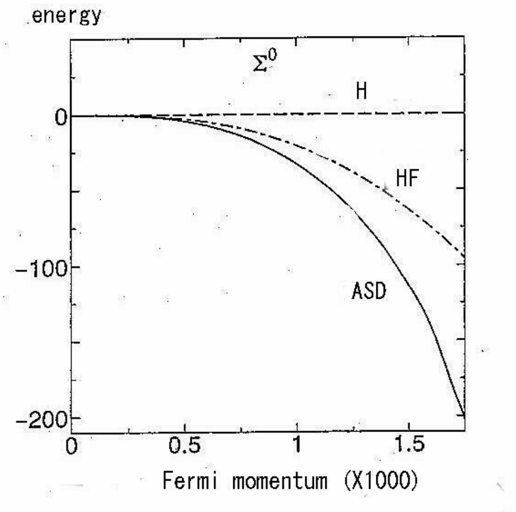

Fig.2 Self-energies for Electron

Reference

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