EFFECTIVE ACTION AND THE ENERGY LEVELS OF HYDROGEN-, HELIUM-, AND LITHIUM-LIKE ATOMS

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Abstract

A systematic derivation of the energy eigenvalue equations for one-, two-, and three-electron atoms is presented in terms of the effective action. By using this method, one can naturally include the field theoretical corrections into the wave equations.

1. Introduction

In this talk we present an application of the generalized on-shell condition,[1),2)] which is obtained by the second derivative of the effective action, and we want to start with a quick review of this formalism. The talk is based on the work with R.Fukuda.[3)]

For simplicity, let us consider the scalar field $\Phi(x)$ and the Lagrangian density $L(\Phi)$ of a system. The generating functional $W[J]$ of the connected Green's function is introduced as

$$\exp(iW[J]) = \int [d\Phi] \exp[\, i\int_{-\infty}^{+\infty} d^4x \, (\, L(\Phi) + J(x)\Phi(x)\,)\,], \tag{1}$$

and the effective action $\Gamma[\phi]$ is defined by the Legendre transformation,

$$\Gamma[\phi] \equiv W[J] - \int d^4x \, J(x)\phi(x), \tag{2}$$

$$\phi(x) \equiv \delta W[J]/\delta J(x). \tag{3}$$

The stationary condition,

$$\delta\Gamma[\phi]/\delta\phi(x) = -J(x) \equiv 0, \tag{4}$$

determines the ground state expectation value of $\Phi(x)$, $<\Phi(x)>_{J=0} \equiv \phi^{(0)}(x)$. We then look for another solution of (4) in the form of $\phi(x)= \phi^{(0)}(x)+\Delta\phi(x)$ and, by assuming $\Delta\phi(x)$ is small, we find the following eigenvalue equation for $\Delta\phi(y)$ (the generalized on-shell condition),

$$\int d^4y \left[\frac{\delta^2\Gamma[\phi]}{\delta\phi(x)\delta\phi(y)} \right]_0 \Delta\phi(y) = 0, \tag{5}$$

where $[\ ]_0$ denotes the value of $[\ ]$ evaluated at $\phi(x)=\phi^{(0)}(x)$.

If we take the space-time translational-invariant case, the zero of the kernel in (5) coincides with the pole of the Green's function by the relation,

$$\int d^4y \left[\frac{\delta^2\Gamma[\phi]}{\delta\phi(x)\delta\phi(y)} \right]_0 \left[\frac{\delta^2 W[J]}{\delta J(y)\delta J(z)} \right]_{J=0} = -\delta^4(x-z). \tag{6}$$

So, eq.(5) determines the particle spectrum or the mode. In the same way, if we study the case where the time-independent external field exists (e.g. the nuclear Coulomb field), eq.(5) is expected to determine the energy eigenvalue and its eigenfunction ($\propto\Delta\phi(x)$) of the excited level. We utilize this fact and study the systematical derivation of the equations that determine the energy levels of hydrogen-, helium-, and lithium-like atoms.

2. One-Electron Atoms

We consider QED under the external field and use the Lagrangian density of the form,

$$L_J \equiv -\frac{1}{4} F_{\mu\nu}F^{\mu\nu} + \overline{\psi}(i\partial\!\!\!/ - m - eA\!\!\!/)\psi - j_\mu A^\mu + J^A_\mu A^\mu + J_\psi \psi + J_{\overline{\psi}} \overline{\psi}, \tag{7}$$

where $j(x) \equiv (\, Z|e|\delta^3(\boldsymbol{x}) \,,\, 0,\, 0,\, 0\,)$ is the source of the nuclear Coulomb field with the atomic number Z. The last three source terms are used as probes. If we want to discuss the finite nuclear size and/or the nuclear magnetic moment, they can be included as the modification of j_μ. Here we notice that the term $J_\psi \psi$ (or $J_{\overline{\psi}} \overline{\psi}$) is necessary for the investigation of the one fermion-number channel, while the term $J^A_\mu A^\mu$ is used for convenience.

The effective action Γ can be obtained with the help of the Legendre transformation formula given by De Dominicis and Martin [4] but with a small modification. For the Grassmann variables, we employ the following definitions of Γ and its functional derivatives,[5]

$$\Gamma[\phi_i] \equiv W[J_i] - J_i\phi_i \qquad (\, \phi_i \equiv \frac{\overrightarrow{\delta}}{\delta J_i} W[J_i] \,), \tag{8}$$

$$\overleftarrow{\delta}\Gamma[\phi_i]/\delta\phi_i = -J_i. \tag{9}$$

The expression of Γ is then summarized as follows,

$$\Gamma[<A>,<\psi>,<\overline{\psi}>] \equiv W[\, J^A,\, J_\psi,\, J_{\overline{\psi}}\,] - J^A \frac{\delta W}{\delta J^A} - J_\psi \frac{\overrightarrow{\delta} W}{\delta J_\psi} - J_{\overline{\psi}} \frac{\overrightarrow{\delta} W}{\delta J_{\overline{\psi}}}$$

$$= \frac{1}{2}<A^\mu> iD_0^{-1}{}_{\mu\nu} <A^\nu> + <\overline{\psi}_i> iS_0^{-1}{}_{ij} <\psi_j> - j_\mu <A^\mu> - i\kappa^{(1)}, \tag{10}$$

where D_0 (S_0) is the bare photon (electron) propagator and $\kappa^{(1)}$ denotes the sum of the one-particle irreducible (1-PI) vacuum diagrams. Graphically $<\psi>$, $<\overline{\psi}>$, and $<A^\mu>$ are expressed by the broken lines which directly connect to the vertices (Fig.1).

As the solution of the stationary condition of Γ, we can choose $<\psi>=<\overline{\psi}>=0$ and, after substituting them, the on-shell condition for $\Delta<\psi>$ is obtained in the following form,

$$\left(S_0^{-1}{}_{ij} + \left[\frac{\overleftarrow{\delta}}{\delta<\psi_j>} \left(\frac{\overleftarrow{\delta}\kappa^{(1)}}{\delta<\overline{\psi}_i>} \right) \right]_0 \right) \Delta<\psi_j> = 0. \tag{11}$$

This is the equation that determines the full energy levels of the hydrogen-like atoms. For example, if we concentrate ourselves on the tree diagram of $\kappa^{(1)}$, we get $<A^\mu> = -iD_0^{\mu\nu} j_\nu \equiv A_c^\mu$ as the stationary solution and eq.(11) becomes,

$$\left[i\partial\!\!\!/_x - m + \gamma_0 \frac{Ze^2}{4\pi|\boldsymbol{x}|} \right] \Delta<\psi>_x = 0. \tag{12}$$

This is nothing but the Dirac equation under the Coulomb potential. In the same way, if we choose the diagrams shown in Fig.1, the lowest-order radiative corrections are properly taken into account and we get the modified Dirac equation from (11) as

$$\left[i\partial\!\!\!/ - m - \Sigma - eA_c^\mu \left\{ \gamma_\mu + \overline{\omega}_{\mu\rho} D_0^{\rho\sigma} \gamma_\sigma + \Lambda_\mu \right\} \right] \Delta<\psi> = 0, \tag{13}$$

where $\overline{\omega}_{\mu\rho}$, $-i\Sigma$, and $-ie\Lambda_\mu$ denote the lowest-order contribution of the vacuum polarization, the electron self-energy, and the vertex correction, respectively. In this way, we can systematically include the quantum field theoretical corrections into the relativistic wave equation.

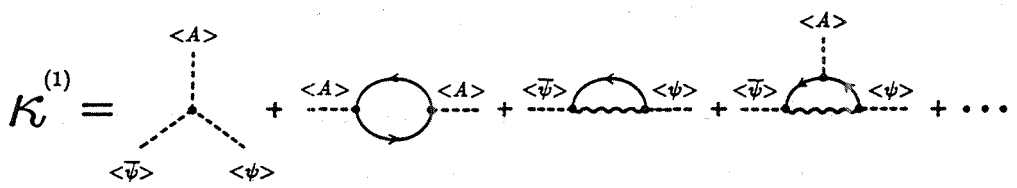

Fig.1 Some of the diagrams included in $\kappa^{(1)}$, which contribute to the modified Dirac equation (13). The wavy line is the photon propagator. The solid line with an arrow denotes the electron one.

3. Two- and Three-Electron Atoms

Next we consider the helium- and lithium-like atoms. In the case of the helium-like atoms, we start with the Lagrangian density (7) plus new source term $(1/2!)K(a,b)\Phi(a)\Phi(b)$ where $\Phi \equiv [\ \psi,\ \overline{\psi},\ A\ ]$ and a,b denote the species of the fields as well as the other degrees of freedom. (Summations over the repeated indices are implied.) In the same way, for the lithium-like atoms, we further use the source term $(1/3!)M(a,b,c)\Phi(a)\Phi(b)\Phi(c)$. Each source is to be antisymmetrized for Grassmann components and to be symmetrized for the others. We notice that the sources $K(\psi,\psi)$ $(,K(\overline{\psi},\overline{\psi}))$ and $M(\psi,\psi,\psi)$ $(,M(\overline{\psi},\overline{\psi},\overline{\psi}))$ are necessary for the investigations of two and three fermion-number channels. Other sources are employed in order to use the (modified) De Dominicis-Martin rules. For the new arguments of Γ, we introduce the notations $<ab>$ and $<abc>$. They are defined as the connected part of $2!\,\overrightarrow{\delta}\,W/\delta K(a,b)$ and $3!\,\overrightarrow{\delta}\,W/\delta M(a,b,c)$, respectively.

As the stationary solutions, $<\psi>$, $<\overline{\psi}>$, $<\psi\psi>$, $<\overline{\psi}\,\overline{\psi}>$, $<\psi\psi\psi>$, $<\overline{\psi}\,\overline{\psi}\,\overline{\psi}>$, and other variables which couple to them can be set equal to zero. Then we get the on-shell conditions in the form of the Nambu-Bethe-Salpeter type wave equations. The result is summarized for helium-like atoms,

$$\frac{1}{2!}\,S^{-1}_{jk}\,S^{-1}_{il}\Delta<\psi_k\psi_l> = [\ \frac{\delta}{\delta<\psi_k\psi_l>}\,(\frac{\delta\ \kappa^{(2)}}{\delta<\overline{\psi}_i\overline{\psi}_j>})\ ]_0\ \Delta<\psi_k\psi_l>, \tag{14}$$

and for lithium-like atoms,

$$\frac{1}{3!}\,S^{-1}_{ii'}\,S^{-1}_{jj'}\,S^{-1}_{kk'}\Delta<\psi_{i'}\psi_{j'}\psi_{k'}>$$

$$= [\ \frac{\overleftarrow{\delta}}{\delta<\psi_{i'}\psi_{j'}\psi_{k'}>}\,(\frac{\overleftarrow{\delta}\,\kappa^{(3)}}{\delta<\overline{\psi}_i\overline{\psi}_j\overline{\psi}_k>})\ ]_0\ \Delta<\psi_{i'}\psi_{j'}\psi_{k'}>, \tag{15}$$

where S_{ij} denotes the full fermion propagator (*i.e.* the stationary solution of $<\psi_i\overline{\psi}_j>$). In (14), $\kappa^{(2)}$ represents the sum of the one- and two-particle irreducible (1,2-PI) vacuum diagrams constructed out of $<a>$, $<ab>$ (propagator), and the

original QED vertex. Similarly, $\kappa^{(3)}$ in (15) denotes the sum of the one-, two-, and three-particle irreducible (1,2,3-PI) vacuum graphs made up of $<a>$, $<ab>$, and $<abc>$. Graphically, each $<abc>$ is represented by the full vertex with the full propagators.[5] The term "three-particle irreducible (3-PI)" usually means the graphs which cannot be disconnected by cutting any three internal lines. But even when the graph is disconnected by this process, if one (and only one) of the disconnected part is the full vertex itself, we also call it the 3-PI graph by the conventions adopted in Ref.4.

4. Comments

Nuclear recoil corrections can be included into our formalism by considering the on-shell condition for $\Delta<\psi_N\,\psi\cdots\psi>$, where ψ_N denotes the nucleon field operator and ψ is that of the electron.

Our method is also available for the non-relativistic models. For example, we can derive the Schrödinger equation under the external potential instead of the Dirac equation (12). The extensions for other cases are straightforward.

References

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