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Time-dependent functional Schrödinger picture approach to many-particle systems

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Abstract

A time-dependent many-body theory for many-particle systems is formulated using the functional Schrödinger picture. Taking a Gaussian trial wave functional and using the variational principle, the equations of motion are obtained. The equations of motion are solved in the small oscillation regime to yield the generalized RPA results. The electron–hole excitation, the collective plasma oscillation for the paramagnetic state, the Stoner excitation and the spin wave for the ferromagnetic state are derived and discussed. As a further test on the versatility of the present method, the formalism is applied to the bound states of the exciton problem and shown to yield the governing equation in a straightforward manner.

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1. Introduction

The time-dependent variational method has been shown to be a promising scheme to investigate problems beyond the mean field in field theories [1, 2]. Also, it is shown that the Schrödinger picture coupled with the variational principle offers a convenient mean in obtaining nonperturbative information from various quantum field theories [3–5]. Recently, there has been some interest in the application of the Schrödinger picture to many-body phenomena [6, 7] in which the functional Schrödinger picture (FSP) has been successfully applied to the interacting electron–gas system and the BCS superconductivity at both zero and finite temperatures to obtain the Hartree–Fock results. However, it appears that the time-independent variational method using a Gaussian trial wave functional does not go beyond

the mean field results, unless more elaborate schemes coupling variational and perturbation methods are employed [8–10]. Another important direction of the theory to be explored is the dynamic aspect of the theory, which is expected to provide dynamic and higher-order information of the system [2]. One example of such an effort is the coupled cluster method (CCM) developed earlier and applied to correlated interacting systems [11]. The CCM was generalized into a full dynamical theory for time-dependent properties by allowing the CCM amplitudes to depend on time and imposing the time-dependent Schrödinger equation [12]. However, we note that the present method does not employ correlated ground state as in the CCM. Instead we directly use the time-dependent Lagrangian formalism to obtain the time-dependent set of equations. We show that this formalism leads into a novel parametrization of the problem, which can be utilized to solve the correlated interacting systems.

2. A time-dependent formulation of the FSP method

In this paper, we present a time-dependent FSP formulation of many-particle systems which leads to the generalized RPA results for the interacting electron–gas system.

For a time-dependent quantum system, the effective action functional is given by

$$S = \int \mathrm{d}t \, L(t) \tag{1}$$

with the effective Lagrangian,

$$L(t) = \langle \psi, t | \left[i \frac{\delta}{\delta t} - \hat{H} \right] | \psi, t \rangle.$$
⁽²⁾

Here, $|\psi, t\rangle$ is the quantum state of the system and \hat{H} is the Hamiltonian of the model. For the interacting electron–gas system, the Hamiltonian is

$$\hat{H} = \sum_{\alpha} \int d^3x \, \hat{\psi}^{\dagger}_{\alpha}(\vec{x}) \left[-\frac{\hbar^2}{2m} \nabla^2 \right] \hat{\psi}_{\alpha}(\vec{x}) + \frac{1}{2} \sum_{\alpha,\beta} \int d^3x \, d^3y \, V(\vec{x},\vec{y}) \hat{\psi}^{\dagger}_{\alpha}(\vec{x}) \hat{\psi}^{\dagger}_{\beta}(\vec{y}) \hat{\psi}_{\beta}(\vec{y}) \hat{\psi}_{\alpha}(\vec{x}) \equiv \sum_{A,B} h_{AB} \hat{\psi}^{\dagger}_{A} \hat{\psi}_{B} + \frac{1}{2} \sum_{A,B} V_{AB} \hat{\psi}^{\dagger}_{A} \hat{\psi}^{\dagger}_{B} \hat{\psi}_{B} \hat{\psi}_{A}.$$
(3)

Here, the last line was introduced for notational convenience. In order to compute *S*, we need a trial wave functional describing the system. In the Floreanini–Jackiw formalism [13], the action of the operators $\hat{\psi}^{\dagger}$ and $\hat{\psi}$ is realized, respectively, by

$$\hat{\psi}_{A}^{\dagger}|\psi,t\rangle \longrightarrow \frac{1}{\sqrt{2}} \left[u_{A}^{\dagger} + \frac{\delta}{\delta u_{A}} \right] \Psi[u,u^{\dagger},t]
\hat{\psi}_{A}|\psi,t\rangle \longrightarrow \frac{1}{\sqrt{2}} \left[u_{A} + \frac{\delta}{\delta u_{A}^{\dagger}} \right] \Psi[u,u^{\dagger},t].$$
(4)

As an approximation, we take a Gaussian trial wave functional

$$\Psi[u, u^{\dagger}, t] = e^{u^{\dagger}Gu}.$$
(5)

Its dual becomes

$$\bar{\Psi}[u, u^{\dagger}, t] = \frac{1}{\text{Det}\left[G + \bar{G}\right]} e^{u^{\dagger} \bar{G} u}$$
(6)

. .

where
$$G = [G^{\dagger}]^{-1}$$
. Using the relation
 $\langle \psi, t | i \frac{\delta}{\delta t} | \psi, t \rangle = \int Du Du^{\dagger} \bar{\Psi}[u, u^{\dagger}, t] i \frac{\delta}{\delta t} \Psi[u, u^{\dagger}, t] = \sum_{A,B} i \dot{G}_{AB} \Sigma_{BA}$
(7)

where $\Sigma = [G + \overline{G}]^{-1}$, one obtains the following expression for the action:

$$S = \int dt \left[\sum_{A,B} i \dot{G}_{AB} \Sigma_{BA} - H \right]$$
(8)

where

$$H = \langle \psi, t | \hat{H} | \psi, t \rangle. \tag{9}$$

The canonical nature of the variational parameters G and $i\Sigma$ leads to the Hamiltonian equations,

$$i\dot{G}_{AB} = \frac{\delta H}{\delta \Sigma_{BA}} \tag{10}$$

$$\mathrm{i}\dot{\Sigma}_{AB} = -\frac{\delta H}{\delta G_{BA}}.\tag{11}$$

The effective Hamiltonian defined by equation (9) can be expressed in terms of G and Σ using equations (3) and (7). After applying some algebra, one obtains

$$H = \frac{1}{2} \sum_{A,B} h_{AB} \Omega_{BA} + \frac{1}{8} \sum_{A,B} V_{AB} \Omega_{AA} \Omega_{BB} - \frac{1}{8} \sum_{A,B} V_{AB} \Omega_{AB} \Omega_{BA}$$
(12)

where

$$\Omega = I + G + \Sigma + G\Sigma - \Sigma G - G\Sigma G \tag{13}$$

and *I* represents the identity matrix. One obtains full equations of motion by using equations (10) and (11). The procedure leading to equation (10)–(13) is completely general. Therefore, we can obtain the corresponding Hamiltonian equation and the parametrized Hamiltonian for any physical Hamiltonian. One such example is the superconductivity channel which is obtained from equation (3). We can readily obtain the corresponding Hamiltonian and exact solution in this case [15]. But due to the complicated nature of the equations, explicit analytic solutions cannot be obtained in general.

3. The small oscillation approximation

It is known that small time-dependent Hartree–Fock fluctuation around the Hartree–Fock ground state yields the RPA results [2, 14]. Here, we show that the present formalism allows one to obtain the generalized RPA results. We introduce small fluctuations,

$$G(t) = \bar{G} + \delta G(t) \qquad \Sigma(t) = \bar{\Sigma} + \delta \Sigma(t) \tag{14}$$

where \bar{G} and $\bar{\Sigma}$ are the static ground state values. Using the above assumptions, the Hamiltonian can be written as follows:

$$H = H^{(0)} + H' \tag{15}$$

where

$$H^{(0)} = \frac{1}{2} \sum_{A,B} h_{AB} \bar{\Omega}_{BA} + \frac{1}{8} \sum_{A,B} V_{AB} [\bar{\Omega}_{AA} \bar{\Omega}_{BB} - \bar{\Omega}_{AB} \bar{\Omega}_{BA}]$$
(16)

$$H' = \frac{1}{2} \sum_{A,B} h_{AB} \delta \Omega_{BA} + \frac{1}{4} \sum_{A,B} V_{AB} [\bar{\Omega}_{AA} \delta \Omega_{BB} - \bar{\Omega}_{AB} \delta \Omega_{BA}] + \frac{1}{8} \sum_{A,B} V_{AB} [\delta \Omega_{AA} \delta \Omega_{BB} - \delta \Omega_{AB} \delta \Omega_{BA}]$$
(17)

and

$$\delta\Omega = \delta\Omega^{(1)} + \delta\Omega^{(2)} = \delta G + \delta G \bar{\Sigma} - \bar{\Sigma} \delta G - \delta G \bar{\Sigma} \bar{G} - \bar{G} \bar{\Sigma} \delta G + \delta \Sigma + \bar{G} \delta \Sigma - \delta \Sigma \bar{G} - \bar{G} \delta \Sigma \bar{G} + \delta G \delta \Sigma - \delta \Sigma \delta G - \delta G \delta \Sigma \bar{G} - \bar{G} \delta \Sigma \delta G - \delta G \bar{\Sigma} \delta G.$$
(18)

In equation (18), $\delta\Omega$ is expressed up to the second order which is sufficient to investigate the linear response. If one is interested in non-linear dynamics, one should include the third-order term as follows:

$$\delta\Omega^{(3)} = -\delta G \delta \Sigma \delta G. \tag{19}$$

When this term is included in the Hamiltonian, it is not possible to solve the equations analytically and, thus, one should resort to numerical calculations. Another way of calculating higher order terms is using a variational perturbation theory or the CCM [9–12]. One notes that $H^{(0)}$ does not contain any time-dependent term and, thus, represents the total energy of the system in the static Hartree–Fock approximation. Using equations (10), (11) and (17), one can obtain the following linear equations of motion in the momentum space:

$$i\delta \dot{G}_{\alpha\beta}(\vec{p}+\vec{q},\vec{p},t) = A_{\alpha\beta}(\vec{p}+\vec{q},\vec{p})\omega_{\alpha\beta}(\vec{p}+\vec{q},\vec{p})\delta G_{\alpha\beta}(\vec{p}+\vec{q},\vec{p},t) + \frac{1}{2}V(\vec{q})\delta_{\alpha\beta}\sum_{\gamma}\int dK\,\delta\Omega_{\gamma\gamma}(\vec{k},\vec{k}-\vec{q},t) - \frac{1}{2}[1+A+B]_{\alpha\beta}(\vec{p}+\vec{q},\vec{p},t)\int dK\,V(\vec{k}-\vec{p})\delta\Omega_{\alpha\beta}(\vec{k},\vec{k}-\vec{q},t)$$
(20)

$$i\delta \dot{\Sigma}_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}, t) = B_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p})\omega_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p})\delta\Sigma_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}, t) + \frac{1}{4}[A - B]_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p})\omega_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p})\delta G_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}, t) - \frac{1}{4}[A - B]_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p})\int dK V(\vec{k} - \vec{p})\delta\Omega_{\alpha\beta}(\vec{k}, \vec{k} - \vec{q}, t)$$
(21)

where

$$dK = \frac{d^3k}{(2\pi^3)} \qquad \omega_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}) = \epsilon_{\alpha}(\vec{p} + \vec{q}) - \epsilon_{\beta}(\vec{p})$$

$$\epsilon_{\alpha}(\vec{p}) = \frac{\hbar^2 p^2}{2m} + nV(0) - \int dK' V(\vec{p} - \vec{k}')\theta(k_{F\alpha} - k') \qquad (22)$$

$$A_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}) = \theta(|\vec{p} + \vec{q}| - k_{F\alpha})\theta(k_{F\beta} - p)$$

$$B_{\alpha\beta}(\vec{p} + \vec{q}, \vec{p}) = \theta(k_{F\alpha} - |\vec{p} + \vec{q}|)\theta(p - k_{F\beta})$$

and

$$\delta\Omega = (A - B)\delta G + 4B\delta\Sigma. \tag{23}$$

The expression of the effective Hamiltonian allows one to write $\delta\Omega$ as follows:

$$\delta\Omega_{\alpha\beta}(\vec{p}+\vec{q},\vec{p}) = \langle \hat{\psi}_{\alpha}^{\dagger}(\vec{p}+\vec{q})\hat{\psi}_{\beta}(\vec{p})\rangle - \bar{\Omega}_{\alpha\beta}(\vec{p}+\vec{q},\vec{p}).$$
(24)

The above equation shows that the diagonal part of $\delta\Omega$ represents the number fluctuation and the off-diagonal part spin fluctuation. Therefore, it is more convenient and physically

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transparent to express the equations of motion in terms of $\delta\Omega$ than δG or $\delta\Sigma$. Using equations (20), (21) and (23), one readily obtains

$$i\delta\dot{\Omega}_{\alpha\beta}(\vec{p}+\vec{q},\vec{p},t) = \omega_{\alpha\beta}(\vec{p}+\vec{q},\vec{p})\delta\Omega_{\alpha\beta}(\vec{p}+\vec{q},\vec{p},t) + \frac{1}{2}[A-B]_{\alpha\beta}(\vec{p}+\vec{q},\vec{p})V(\vec{q})\delta_{\alpha\beta}\sum_{\gamma}\int dK\,\delta\Omega_{\gamma\gamma}(\vec{k},\vec{k}-\vec{q},t) - [A-B]_{\alpha\beta}(\vec{p}+\vec{q},\vec{p})\int dK\,V(\vec{k}-\vec{p})\delta\Omega_{\alpha\beta}(\vec{k},\vec{k}-\vec{q},t).$$
(25)

This equation provides a formal basis to discuss physical properties of the electron gas. First, we consider the diagonal parts of $\delta\Omega$ which represents the paramagnetic case and define the diagonal part as follows:

$$\delta\Omega_{\alpha\alpha} = \delta\rho. \tag{26}$$

Using this expression, we obtain

$$\begin{split} \mathrm{i}\delta\dot{\rho}(\vec{p}+\vec{q},\vec{p},t) &= \omega_{\alpha\alpha}(\vec{p}+\vec{q},\vec{p})\delta\rho(\vec{p}+\vec{q},\vec{p},t) \\ &+ [A-B]_{\alpha\alpha}(\vec{p}+\vec{q},\vec{p})V(\vec{q})\int\mathrm{d}K\,\delta\rho(\vec{k},\vec{k}-\vec{q},t) \\ &- [A-B]_{\alpha\alpha}(\vec{p}+\vec{q},\vec{p})\int\mathrm{d}K\,V(\vec{k}-\vec{p})\delta\rho(\vec{k},\vec{k}-\vec{q},t). \end{split}$$
(27)

The above equation is known as the generalized, or extended RPA, which contains the exchange terms in the particle–hole excitation energy $\omega_{\alpha\alpha}$ [16].

4. Physical properties of the electron gas and application to the exciton problem

Although substantially simplified, it is still impossible to solve the above equation analytically. Neglecting the exchange contribution, one obtains the well-known RPA result,

$$i\delta\dot{\rho}(\vec{p}+\vec{q},\vec{p},t) = \omega_0^{ph}(\vec{p}+\vec{q},\vec{p})\delta\rho(\vec{p}+\vec{q},\vec{p},t) + [A-B](\vec{p}+\vec{q},\vec{p})V(\vec{q})\int dK\,\delta\rho(\vec{k},\vec{k}-\vec{q},t)$$
(28)

where $\omega_0^{ph}(\vec{p} + \vec{q}, \vec{p}) = \epsilon_0(\vec{p} + \vec{q}) - \epsilon_0(\vec{p})$ is the particle-hole excitation energy for the non-interacting system. Assuming a solution

$$\delta\rho(\vec{p}+\vec{q},\vec{p},t) = \delta\rho^{(0)}(\vec{p},\vec{q})e^{-i\omega_q t}$$
⁽²⁹⁾

one obtains

$$\omega_{q}\delta\rho^{(0)}(\vec{p}+\vec{q},\vec{p}) = \omega_{0}^{ph}(\vec{p}+\vec{q},\vec{p})\delta\rho^{(0)}(\vec{p}+\vec{q},\vec{p}) + [A-B](\vec{p}+\vec{q},\vec{p})V(\vec{q})\int dK\,\delta\rho^{(0)}(\vec{k},\vec{k}-\vec{q}).$$
(30)

It is convenient to rewrite the above equation as an integral equation,

$$\delta\rho^{(0)}(\bar{p}', \vec{p}, \vec{q}; \omega_q) = \gamma \,\delta(\vec{p} - \bar{p}') + G_0^{ph}(\vec{p}, \vec{q}; \omega_q) V(\vec{q}) \int \mathrm{d}K \,\delta\rho^{(0)}(\bar{p}', \vec{k}, \vec{q}; \omega_q) \tag{31}$$

where γ stands for a phase factor to keep $\delta \rho^{(0)}$ real. The particle–hole Green's function for the non-interacting system G_0^{ph} is defined as follows:

$$G_0^{ph}(\vec{p}, \vec{q}; \omega_q) = \frac{A}{\omega_q - \omega_0^{ph} + i\eta} - \frac{B}{\omega_q - \omega_0^{ph} - i\eta}.$$
(32)

Then, $\int dK \,\delta\rho^{(0)}(\vec{k},\vec{q})$ can be found by integrating equation (31) with respect to \vec{p} ,

$$\int dK \,\delta\rho^{(0)}(\vec{k},\vec{q}) = \frac{\gamma}{1 - V(\vec{q})D_0(\vec{q};\omega_q)}$$
(33)

where the polarization function is defined by

$$D_0(\vec{q};\omega_q) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3} G_0^{ph}(\vec{p},\vec{q};\omega_q).$$
(34)

Substituting equation (33) back into equation (31) yields

$$\delta\rho^{(0)}(\vec{p}', \vec{p}, \vec{q}; \omega_q) = \gamma \left[\delta(\vec{p} - \vec{p}') + \frac{G_0^{ph}(\vec{p}, \vec{q}; \omega_q)V_q}{1 - V_q D_0(\vec{q}; \omega_q)} \right].$$
 (35)

Since the poles of $\delta \rho^{(0)}$ give the excited states of the system, the excited states in the RPA occur at ω^q such that

$$1 = V_q D_0(\vec{q}; \omega_q). \tag{36}$$

The above result is the well-known RPA dispersion relation for the collective modes of an interacting fermion system [2].

Next, we consider the off-diagonal part of $\delta\Omega$, which represents the magnetic excitations,

$$\delta\Omega_{\uparrow\downarrow} = \delta\Omega_{\downarrow\uparrow}^{\dagger} = \delta\sigma. \tag{37}$$

Substituting this expression into equation (25), one obtains

$$\begin{split} \mathrm{i}\delta\dot{\sigma}\left(\vec{p}+\vec{q},\,\vec{p},t\right) &= \omega_{\uparrow\downarrow}(\vec{p}+\vec{q},\,\vec{p})\delta\sigma\left(\vec{p}+\vec{q},\,\vec{p},t\right) \\ &+ [A-B]_{\uparrow\downarrow}(\vec{p}+\vec{q},\,\vec{p})\int\mathrm{d}K\,\delta V\left(\vec{k}-\vec{p}\right)\delta\sigma\left(\vec{k},\,\vec{k}-\vec{q},t\right). \end{split} \tag{38}$$

One notes that the direct Coulomb term disappears naturally, thus showing that the direct Coulomb interaction is not related with the ferromagnetic state. Although the above equation is similar to equation (28), it is not possible to solve it analytically since the exchange interaction is contained in the integral. We approximate the integration part of the last term of equation (38) as

$$\int \mathrm{d}K \, V(\vec{k} - \vec{p}) \delta\sigma(\vec{k}, \vec{k} - \vec{q}, t) \approx \tilde{V}(\vec{q}) \int \mathrm{d}K \, \delta\sigma(\vec{k} + \vec{q}, \vec{k}, t) \tag{39}$$

using the result of the average theorem of the integration [16]. It is noted that $\tilde{V}(\vec{q})$ represents the average magnitude of the exchange interaction. With this approximation, equation (38) assumes the same form as equation (28). Following the same steps, we obtain

$$\delta\sigma^{(0)}(\bar{p}',\bar{p},\bar{q};\omega_q) = \gamma \left[\delta(\bar{p}-\bar{p}') + \frac{G_{\uparrow\downarrow}(\bar{p},\bar{q};\omega_q)}{1-\tilde{V}_q D_{\uparrow\downarrow}(\bar{q};\omega_q)} \right]$$
(40)

where

$$G_{\uparrow\downarrow}(\vec{p},\vec{q};\omega_q) = \frac{A_{\uparrow\downarrow}}{\omega_q - \omega_{\uparrow\downarrow} + i\eta} - \frac{B_{\uparrow\downarrow}}{\omega_q - \omega_{\uparrow\downarrow} - i\eta}$$
(41)

$$D_{\uparrow\downarrow}(\vec{q};\omega_q) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3} G_{\uparrow\downarrow}(\vec{p},\vec{q};\omega_q).$$
(42)

The magnetic excitations occur when

$$1 = V(\vec{q})D_{\uparrow\downarrow}(\vec{q};\omega_q) \tag{43}$$

is satisfied. The above equations give the Stoner excitation energy modified by the forcing term and the spin-wave excitation energy [16].

In the above, we have shown that the present formalism offers a convenient tool to handle interacting fermion systems. As an another example of the present approach, we now consider the exciton problem. In this case, the subscripts α and β in equation (25) represent the band indices. Since spin is not important in treating excitons, equation (25) is transformed as follows:

$$i\delta\dot{\Omega}_{cv}(\vec{p},\vec{q},t) = \left[E_c(\vec{p}) - E_v(\vec{q})\right]\delta\Omega_{cv}(\vec{p},\vec{q},t) -\int dK V(\vec{k}-\vec{p})\delta\Omega_{cv}(\vec{k},\vec{k}-\vec{p}+\vec{q},t)$$
(44)

where c(v) represents the conduction (valence) band. One notes that the direct Coulomb term disappears naturally. This indicates the importance of the exchange interaction in the exciton states. In real semiconductors, the complex structures of bands do not allow to solve equation (44) analytically. Therefore, we approximate the bands as parabolic as follows:

$$E_{c}(\vec{p}) = \frac{\hbar^{2} p^{2}}{2m_{c}} + E_{g}$$
(45*a*)

$$E_v(\vec{p}) = -\frac{\hbar^2 p^2}{2m_v} \tag{45b}$$

where $m_c (m_v)$ is the conduction electron (valence hole) effective mass and E_g is the energy gap. We choose the top of the valence band as zero, so that the bottom of the conduction band has the energy value of E_g . An effective interaction is taken to be

$$V(k) = \frac{4\pi e^2}{\epsilon k^2} \tag{46}$$

where ϵ is the appropriate dielectric constant. We introduce the total and relative momentum coordinates, given by $\vec{p} - \vec{q} = \vec{Q}'$ and $(\vec{p} + \vec{q})/2 = \vec{q}$, respectively. Using these notations we write the equation of motion in the centre of mass system as follows:

$$i\delta\dot{\Omega}_{cv}(\vec{q},\vec{Q},t) = \left[E_c \left(\vec{q} + \frac{1}{2}\vec{Q} \right) - E_v \left(\vec{q} - \frac{1}{2}\vec{Q} \right) \right] \delta\Omega_{cv}(\vec{q},\vec{Q},t) - \int dK \ V(\vec{k} - \vec{q}) \delta\Omega_{cv}(\vec{k},\vec{Q},t)$$
(47)

where we have deleted the prime from \bar{q}' for convenience. Using parabolic bands in equation (45) and the following expression:

$$\delta\Omega_{cv}(\vec{q},\vec{Q},t) = \delta\Omega_Q^{(0)}(\vec{q})e^{-i\omega_Q t}$$
(48)

we obtain

$$\omega_{Q}\delta\Omega_{Q}^{(0)}(\vec{q}) = \left[\frac{\hbar^{2}q^{2}}{2\mu} + \frac{\hbar^{2}}{2}\left(\frac{1}{m_{c}} - \frac{1}{m_{v}}\right)\vec{q}\cdot\vec{Q} + \frac{\hbar^{2}Q^{2}}{8\mu}\right]\delta\Omega_{Q}^{(0)}(\vec{q}) -\int dK \, V(\vec{k} - \vec{q})\delta\Omega_{Q}^{(0)}(\vec{k})$$
(49)

where μ is the reduced mass given by $1/\mu = 1/m_c + 1/m_v$. Introducing Fourier transformations as

$$\delta\Omega_{\mathcal{Q}}(\vec{k}) = \int d\vec{r} \, \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} \delta\Omega_{\mathcal{Q}}^{(0)}(\vec{r}) \tag{50a}$$

$$V(\vec{k} - \vec{q}) = \int d\vec{r} \, \mathrm{e}^{\mathrm{i}(\vec{q} - \vec{k}) \cdot \vec{r}} \, V(\vec{r})$$
(50b)

one can obtain the governing equation for the exciton state [17],

$$\left[\frac{\hbar^2 q^2}{2\mu} - \frac{e^2}{\epsilon r} - \frac{\hbar^2}{2} \left(\frac{1}{m_v} - \frac{1}{m_c}\right) \vec{q} \cdot \vec{Q}\right] \delta\Omega_Q^{(0)}(\vec{r}) = \left[\omega_Q - E_g - \frac{\hbar^2 Q^2}{8\mu}\right] \delta\Omega_Q^{(0)}(\vec{r})$$
(51)

where $\vec{q} = -i\nabla$ is now an operator. One can easily transform the above equation for the hydrogen-like case and obtain the exciton energies for each Q as follows:

$$\omega_n(Q) = E_g - \frac{\mu e^4}{2\hbar^2 \epsilon^2 n^2} + \frac{\hbar^2 Q^2}{2(m_c + m_v)}.$$
(52)

5. Conclusion

In summary, a time-dependent functional Schrödinger picture theory of many-particle systems is presented. We have obtained dynamic equations for physical variables and the generalized RPA results by expanding around the static Hartree–Fock ground state. Applying the method to the electron gas, we have obtained excitation spectra for the electron–hole excitation, the collective plasma oscillation, the Stoner excitation and the spin wave for the ferromagnetic state. In order to show the convenience and versatility of the present formalism, we have also applied the method to the exciton problem and obtained the generalized equation for the excitonic state.

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