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2009 J. Phys. A: Math. Theor. 42 135301

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A diagrammatic calculation of the energy spectrum of quantum impurity in degenerate Bose–Einstein condensate

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Received 27 May 2008, in final form 30 October 2008

Published 4 March 2009

Online at stacks.iop.org/JPhysA/42/135301

Abstract

In this paper we consider a quantum particle moving through dilute Bose–Einstein condensate at zero temperature. In our formulation the impurity particle interacts with the gas of uncoupled Bogoliubov’s excitations. The perturbation theory for the Green’s function of the impurity particle with respect to the impurity–condensate interaction is constructed by employing the coherent-state path integral approach. The perturbative expansion for the Green’s function is resummed into the expansion for its self-energy part with the help of the diagrammatic technique developed in this work. The dispersion relation for the impurity clothed by condensate excitations is obtained and effective mass is evaluated beyond the Golden rule approximation.

PACS numbers: 03.75.Nt, 03.75.Kk, 31.15.xk, 31.15.xp, 31.15.xm

1. Introduction

A significant number of theoretical works have been devoted to the quantum theory of superfluidity on a microscopic scale. Recent interest stems from several new experiments on the superfluid helium and other Bose–Einstein condensates (BEC). Rotational motion of molecules has been extensively studied in the superfluid helium droplets [1, 2]. A unique property of the measured rotational spectra poses a large number of questions, such as: what is the collective molecule/superfluid wavefunction that describes sharp rotational states observed in experiments; what are the properties of finite systems and how is the limit of a bulk superfluid reached [3]? Similar microscopic phenomena were studied in the BEC of sodium atoms in magnetic traps [4]. A linear motion of impurities was shown to be dissipationless for the speeds below the condensate speed of sound. A large number of theoretical works addressed the molecule–He droplet system using imaginary time path integral Monte-Carlo approaches [5–11]. While in certain cases remarkable agreement with experimental constants was obtained [11], those works are strictly limited to the calculation of statistical properties.

A number of theoretical works considered a real-time dynamics of an impurity in dilute BEC. A macroscopic particle interacting with dilute BEC has been considered [12]. In this case the motion of the particle is equivalent to the BEC in a time-dependent external potential. This problem was treated by solving time-dependent Gross–Pitaevskii equations [13]. A microscopic particle interacting with the dilute BEC in Bogoliubov’s approximation has been considered by several authors using general Golden rule considerations [14–16]. These works were based on the result of Miller *et al* [17] which was obtained using time-independent perturbation theory. The Bogoliubov’s treatment has also been successfully used for the investigation of the force acting on the impurity particle due to the quantum fluctuations in BEC [18, 19]. Some authors treated a particle strongly interacting with Bogoliubov’s BEC and found a possibility of self-localization [20–22]. In summary, all of the previous works dealt with the lowest order of the perturbation theory, either using the Golden rule approximation or considering the interaction with the fluctuations of the Gross–Pitaevskii field. What we seek is the perturbation theory that can be systematically extended to an arbitrary order. In the present paper we use the field theoretical methods to develop such treatment. The natural way to compute the real-time dynamics of an impurity is to develop an expansion considering particle–BEC interaction as a perturbation. Our previous work [23] as well as several works of other authors [14–17] dealt with the lowest order term that corresponds to the Golden rule limit. In this work we describe an impurity moving through BEC as a microscopic particle within time-dependent perturbation theory. We present the treatment which allows us to evaluate the terms of an arbitrary order of perturbation expansion.

One of the main problems of treating the real-time dynamics within time-dependent perturbation theory is that the phase of the system oscillations can also be shifted due to the perturbation. Expanding directly the result in powers of small parameter one encounters the so-called secular terms in this expansion which have a power-law dependence on time and increase with growing time. Thus, direct perturbation theory fails to work beyond the Golden rule limit at long times. In this work we develop a method which allows us to avoid the appearance of secular terms and consider higher orders of perturbation theory.

This paper is organized as follows: in section 2 we introduce the Hamiltonian of a quantum particle moving within the interacting Bose gas. No assumption is made about the relative mass of an impurity compared to that of the Bose particles. After the introduction of the general Hamiltonian, the Bogoliubov’s approximation is made to convert the Hamiltonian to the diagonal form. Then the problem is reduced to the quantum particle moving through the gas of non-interacting Bogoliubov’s excitations. The time evolution of a bosonic system described by the Hamiltonian in secondary quantized form is written in terms of coherent-state path integral in section 3. Because of the linear dependence of the interaction Hamiltonian on the BEC degrees of freedom this functional integral can be reduced to the non-Gaussian integral over the particle trajectories. The non-Gaussian part describing particle–BEC interaction leads to the formal perturbation expansion constructed in section 4. In order to prevent the appearance of the secular terms, the perturbation series is resummed as an expansion for the poles of the Green’s function with the help of the diagrammatic technique. In this way we obtain the expression for the self-energy part which is responsible for the shift of the Green’s function pole due to the particle–BEC interaction, i.e. the dispersion relation for the impurity dressed by the cloud of BEC excitations. The similar resummation techniques leading to the Dyson’s-type equation for the single particle Green’s function can be found, for example, in [24, 25]. The limit of the energy at small momenta allows us to compute the effective mass of the particle up to an arbitrary order of the perturbation theory. As an example of this technique, in section 5 we compute the term of the perturbation expansion that is next to the Golden rule result and its contribution to the energy spectrum and effective mass of

the particle. The last section gives the conclusion as well as some possible outlooks of our work.

2. Model Hamiltonian

Let us start with the Hamiltonian of interacting Bose particles in secondary quantization representation

$$H_B = \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{2m} b_{\mathbf{p}}^{\dagger} b_{\mathbf{p}} + \frac{1}{2V} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}} U(\mathbf{p}) b_{\mathbf{p}_1 - \mathbf{p}}^{\dagger} b_{\mathbf{p}_2 + \mathbf{p}}^{\dagger} b_{\mathbf{p}_2} b_{\mathbf{p}_1}, \quad (1)$$

where $U(\mathbf{p})$ is the Fourier transform of the interaction potential

$$U(\mathbf{p}) = \int U(\mathbf{r}) e^{i\mathbf{p}\mathbf{r}} d\mathbf{r}. \quad (2)$$

The Plank constant \hbar is set to unity here and throughout this paper. We will concentrate on the case of dilute gas $r_0 \ll n^{-1/3}$ where r_0 is the range of potential on which $U(r)$ differs from zero significantly and n denotes density of gas. So the Fourier transform of the interaction potential $U(\mathbf{p})$ can be replaced by its zero component $U_0 = \int d\mathbf{r} U(\mathbf{r})$, which is connected with the length of s -scattering in the first-order Born approximation as $a_s = mU_0/4\pi$. Then we will consider degenerate gas at zero temperature. In this case the Hamiltonian (1) can be reduced to the diagonal form with the help of the Bogoliubov's method [26]:

$$H_B = E_0 + \sum_{\mathbf{p}} \epsilon(p) B_{\mathbf{p}}^{\dagger} B_{\mathbf{p}}. \quad (3)$$

Here the new bosonic operators $B_{\mathbf{p}}^{\dagger}$ and $B_{\mathbf{p}}$ create and annihilate the collective excitations in BEC with the spectrum

$$\epsilon(p) = \sqrt{\frac{p^2}{2m} \left(\frac{p^2}{2m} + 2nU_0 \right)}, \quad (4)$$

which has the phonon-like behavior at low momenta, i.e. $\epsilon(p \rightarrow 0) = p\sqrt{nU_0/m} = pc$, where c is the speed of sound. The original particle operators $b_{\mathbf{p}}^{\dagger}$ and $b_{\mathbf{p}}$ are connected with the operators of Bogoliubov's excitations $B_{\mathbf{p}}^{\dagger}$ and $B_{\mathbf{p}}$ by the following relations [24, 27]:

$$b_{\mathbf{p}} = \alpha_{\mathbf{p}} B_{\mathbf{p}} + \beta_{\mathbf{p}} B_{-\mathbf{p}}^{\dagger}, \quad b_{\mathbf{p}}^{\dagger} = \alpha_{\mathbf{p}} B_{\mathbf{p}}^{\dagger} + \beta_{\mathbf{p}} B_{-\mathbf{p}}, \quad (5)$$

where the transformation coefficients are

$$\alpha_{\mathbf{p}} = \frac{\mu_{\mathbf{p}}}{\sqrt{\mu_{\mathbf{p}}^2 - 1}}, \quad \beta_{\mathbf{p}} = \frac{1}{\sqrt{\mu_{\mathbf{p}}^2 - 1}}, \quad (6)$$

$$\mu_{\mathbf{p}} = -\frac{\epsilon(\mathbf{p}) + p^2/2m + nU_0}{nU_0}.$$

The ground-state energy of BEC is given by

$$E_0 = \frac{nU_0}{2}(N - 1) + \frac{1}{2} \sum_{\mathbf{p} \neq 0} \left(\epsilon(p) - \frac{p^2}{2m} - nU_0 \right). \quad (7)$$

Next, we will consider a single quantum particle with mass M and momentum \mathbf{q} interacting with the environment of Bose gas discussed above. The whole system is then described by the following Hamiltonian:

$$H = \sum_{\mathbf{q}} \frac{q^2}{2M} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + H_B + H_I \quad (8)$$

with the particle–environment interaction

$$H_I = \frac{g}{V} \sum_{\mathbf{p}, \mathbf{k}, \mathbf{q}} b_{\mathbf{p}+\mathbf{k}}^+ b_{\mathbf{p}} a_{\mathbf{q}-\mathbf{k}}^+ a_{\mathbf{q}}. \quad (9)$$

Here the bosonic operators $a_{\mathbf{q}}^+/a_{\mathbf{q}}$ create/annihilate the particle in state $|\mathbf{q}\rangle$ and the coupling constant g is determined as zero Fourier component of the system–environment interaction. After application of the Bogoliubov’s transformation to the interaction (9) the Hamiltonian of the whole system (8) takes the form

$$H = E'_0 + \sum_{\mathbf{q}} \frac{\mathbf{q}^2}{2M} a_{\mathbf{q}}^+ a_{\mathbf{q}} + \sum_{\mathbf{p}} \epsilon(p) B_{\mathbf{p}}^+ B_{\mathbf{p}} + \sum_{\mathbf{q}, \mathbf{p} \neq 0} \gamma_{\mathbf{p}} (a_{\mathbf{q}-\mathbf{p}}^+ a_{\mathbf{q}} B_{\mathbf{p}}^+ + a_{\mathbf{q}+\mathbf{p}}^+ a_{\mathbf{q}} B_{\mathbf{p}}), \quad (10)$$

$$\gamma_{\mathbf{p}} = \frac{g}{V} \sqrt{\frac{Np^2}{2m\epsilon(p)}}.$$

The ground-state energy $E'_0 = E_0 + gn$ is now shifted with respect to the E_0 due to the system–condensate interaction.

In the interaction part of the Hamiltonian as well as in the Hamiltonian of the free BEC we neglected the terms responsible for the interaction between the Bogoliubov’s excitations. This approximation remains valid if the single impurity alters the surrounding BEC only slightly which is always the case in the macroscopic limit. Below we construct the perturbation theory in powers of coupling strength $\gamma_{\mathbf{p}}$ for the propagator of the relevant particle. While we keep the interaction between BEC particles weak, this perturbative expansion is meaningful up to any order perturbation term in powers of the impurity–BEC interaction. The full expansion is valid as long as the BEC is well described within Bogoliubov’s approximation.

3. Coherent-state path integral formulation of the evolution operator

The main task of the present work is to evaluate the dynamical quantities such as transition amplitudes or Green’s function of the system described by the Hamiltonian in bosonic creation/annihilation operator representation. In order to proceed with such kinds of calculations one can employ the coherent-state path integral technique [28, 29]. In this section we give basic introduction into the coherent-state path integral formulation of the dynamics of the Bose many-particle systems.

First, let us define the coherent state of the many-particle Bose system $|\{z_{\mathbf{p}}\}\rangle = |z_{\mathbf{p}_1}, z_{\mathbf{p}_2}, \dots, z_{\mathbf{p}_k}, \dots\rangle$ as an eigenstate of the annihilation operator, i.e. $\hat{a}_{\mathbf{p}_k} |\{z_{\mathbf{p}}\}\rangle = z_{\mathbf{p}_k} |\{z_{\mathbf{p}}\}\rangle$. One can write the matrix element of the evolution operator in coherent-state basis as the following functional integral [28]:

$$\langle \{z_{\mathbf{p}}\} | e^{-iHt} | \{z'_{\mathbf{p}}\} \rangle = \int D[\{z_{\mathbf{p}}^*(\tau)\}, \{z_{\mathbf{p}}(\tau)\}] \times \exp \left[-\frac{1}{2} \sum_{\mathbf{p}} (|z_{\mathbf{p}}|^2 + |z'_{\mathbf{p}}|^2) - iS(\{z_{\mathbf{p}}(\tau)\}, \{z_{\mathbf{p}}^*(\tau)\}) \right]. \quad (11)$$

Here S denotes the action depending on the trajectories $z_{\mathbf{p}}(\tau)$ and $z_{\mathbf{p}}^*(\tau)$:

$$S(\{z_{\mathbf{p}}(\tau)\}, \{z_{\mathbf{p}}^*(\tau)\}) = i \sum_{\mathbf{p}} z_{\mathbf{p}}^*(t) z_{\mathbf{p}}(t) - \int_0^t d\tau \left[i \sum_{\mathbf{p}} z_{\mathbf{p}}^*(\tau) \dot{z}_{\mathbf{p}}(\tau) - H(\{z_{\mathbf{p}}^*(\tau)\}, \{z_{\mathbf{p}}(\tau)\}) \right], \quad (12)$$

which must be evaluated with the boundary conditions $z_p(0) = z_p'$ and $z_p^*(t) = z_p^*$, where z_p^* and z_p' correspond to the bra and ket states on the left-hand side of equation (11), respectively. The integration in (11) is performed over all trajectories depending on time, and the symbol $D[\dots]$ is defined as

$$D[\{z_p^*(\tau)\}, \{z_p(\tau)\}] = \prod_p \prod_\tau \frac{dz_p^*(\tau) dz_p(\tau)}{\pi}. \quad (13)$$

Here we have to note that the trajectories $z_p^*(\tau)$ and $z_p(\tau)$ are different functions and are not conjugated of each other.

Now let us consider the vacuum amplitude for free Bose gas described by the Hamiltonian $H = \sum_p E(p) a_p^+ a_p$:

$$\langle 0 | \exp \left(-it \sum_p E(p) a_p^+ a_p \right) | 0 \rangle = \int D[\{z_p^*(\tau)\}, \{z_p(\tau)\}] e^{-iS_0}, \quad (14)$$

where S_0 is the free action

$$S_0 = \sum_p \int_0^t d\tau z_p^*(\tau) \hat{G}_p^{-1} z_p(\tau), \quad \hat{G}_p^{-1} = -i \frac{\partial}{\partial \tau} + E(p). \quad (15)$$

Since the vacuum state is defined as $|0\rangle = |\{z_p\} = 0\rangle$, the functional integral (14) has to be evaluated with zero boundary conditions, i.e. $z_p(0) = z_p^*(t) = 0$. Below we will need the so-called generating functional for the vacuum amplitude which is defined by introducing some auxiliary sources $j_p^*(\tau)$ and $j_p(\tau)$ into the action, i.e.

$$\Lambda[\{j_p^*(\tau)\}, \{j_p(\tau)\}] = \int D[\{z_p^*(\tau)\}, \{z_p(\tau)\}] \times \exp \left[-iS_0 + \int_0^t d\tau \sum_p (z_p^*(\tau) j_p^*(\tau) + z_p(\tau) j_p(\tau)) \right]. \quad (16)$$

Note that the sources $j_p^*(\tau)$ and $j_p(\tau)$ as well as the trajectories $z_p^*(\tau)$ and $z_p(\tau)$ are different functions, so they are not conjugated. One can evaluate the above integral employing the background field method [30], i.e. splitting the integral into the factor depending on external sources, and the integral over fluctuations around the background field. After that one obtains the expression for the generating functional

$$\Lambda[\{j_p^*(\tau)\}, \{j_p(\tau)\}] = \exp \left(\sum_p \int_0^t d\tau \int_0^t d\tau' G_p(\tau - \tau') j_p(\tau) j_p^*(\tau') \right), \quad (17)$$

where $G_p(\tau)$ is the Green's function of the operator \hat{G}_p^{-1} :

$$G_p(\tau - \tau') = \Theta(\tau - \tau') \exp[-iE(p)(\tau - \tau')], \quad (18)$$

and $\Theta(\tau)$ denotes the Heaviside step function.

The last point is to determine the mean value of some functional of trajectories $\mathcal{A}[\{z_p(\tau)\}, \{z_p^*(\tau)\}]$ as follows:

$$\langle \mathcal{A} \rangle = \int D[\{z_p^*(\tau)\}, \{z_p(\tau)\}] \mathcal{A} e^{-iS_0}. \quad (19)$$

In the following section, we will have to evaluate the mean products of the trajectories taken at different moments of time which can be written as the functional derivative of the generating

functional:

$$\begin{aligned} & \langle z_{\mathbf{p}_1}(s_1) z_{\mathbf{p}_2}(s_2) \dots z_{\mathbf{p}_n}(s_n) z_{\mathbf{p}_{n+1}}^*(s_{n+1}) z_{\mathbf{p}_{n+2}}^*(s_{n+2}) \dots z_{\mathbf{p}_{2n}}^*(s_{2n}) \rangle \\ &= \frac{\delta^{2n}}{\delta j_{\mathbf{p}_1}(s_1) \delta j_{\mathbf{p}_2}(s_2) \dots \delta j_{\mathbf{p}_n}(s_n) \delta j_{\mathbf{p}_{n+1}}^*(s_{n+1}) \delta j_{\mathbf{p}_{n+2}}^*(s_{n+2}) \dots \delta j_{\mathbf{p}_{2n}}^*(s_{2n})} \Big|_{j_{\mathbf{p}}=j_{\mathbf{p}}^*=0} \\ & \times \Lambda[\{j_{\mathbf{p}}^*(\tau)\}, \{j_{\mathbf{p}}(\tau)\}]. \end{aligned} \quad (20)$$

For example, a single particle Green's function is $\langle z_{\mathbf{p}}(s) z_{\mathbf{p}'}^*(s') \rangle = G_{\mathbf{p}}(s - s') \delta_{\mathbf{p}, \mathbf{p}'}$. Since in the case $s = s'$ the Green's function $G(0) = \langle a^+(s) a(s) \rangle = 0$, the expression (18) must be written in the form $G(s - s') = \Theta(s - s' - 0) \exp[-iE(p)(s - s')]$.

4. The diagrammatic technique for the Green's function of the relevant particle

The purpose of this section is the construction of the perturbation theory for the Green's function of the impurity particle $\mathcal{G}_{\mathbf{p}}(t)$ defined as the correlation function of the creation and annihilation operators, i.e. $\mathcal{G}_{\mathbf{p}}(t) = \langle a_{\mathbf{p}}(t)^+ a_{\mathbf{p}}(0) \rangle$. Let us start with the transition amplitude

$$w_{i \rightarrow f} = \langle 0|_B \langle f| e^{-iHt} |i\rangle |0\rangle_B, \quad (21)$$

which describes the transition of the impurity particle from some initial state $|i\rangle$ to some final state $|f\rangle$ while the BEC remains in its vacuum state $|0\rangle_B$, i.e. state with an absence of Bogoliubov's excitations. It is clear that in this case $|i\rangle = |f\rangle$. Below we will consider the eigenstate of momentum $|\mathbf{p}\rangle$ as the initial and final states of the impurity

$$w_{i=f=|\mathbf{p}\rangle} = \mathcal{G}_{\mathbf{p}} = \langle 0|_B \langle \mathbf{p}| e^{-iHt} |\mathbf{p}\rangle |0\rangle_B. \quad (22)$$

One can write the transition amplitude as the following correlation function:

$$\mathcal{G}_{\mathbf{p}}(t) = \langle 0|_B \langle 0| a_{\mathbf{p}} e^{-iHt} a_{\mathbf{p}}^+ |0\rangle |0\rangle_B = \langle a_{\mathbf{p}}(t) a_{\mathbf{p}}^+(0) \rangle. \quad (23)$$

Here $|0\rangle$ denotes the state of the impurity with no particle and the brackets $\langle \dots \rangle$ mean averaging over vacuum states of the BEC and the impurity. Thus we see that the transition amplitude of the form (22) coincides with the Green's function of the impurity, and its poles determine the excitation spectrum of the particle interacting with the surrounding BEC. Now we can employ the path integral formulation of the matrix element of the evolution operator developed in section 3:

$$\begin{aligned} \mathcal{G}_{\mathbf{p}}(t) &= \int D[\{a_{\mathbf{q}}^*(\tau)\}, \{a_{\mathbf{q}}(\tau)\}] a_{\mathbf{p}}(t) a_{\mathbf{p}}^*(0) \int D[\{b_{\mathbf{q}}^*(\tau)\}, \{b_{\mathbf{q}}(\tau)\}] \\ & \times \exp \left[-iS_P - iS_B - i \int_0^t d\tau \sum_{\mathbf{q}, \mathbf{q}' \neq 0} \gamma_{\mathbf{q}} (a_{\mathbf{q}'-\mathbf{q}}^*(\tau) a_{\mathbf{q}'}(\tau) b_{\mathbf{q}}^*(\tau) + a_{\mathbf{q}'+\mathbf{q}}^*(\tau) a_{\mathbf{q}}(\tau) b_{\mathbf{q}}(\tau)) \right], \end{aligned} \quad (24)$$

where we have determined the action of the free impurity particle S_P and the action of the free particle in BEC S_B the same way as the free action S_0 in equation (15). Since the interaction part of the action in the functional integral (24) has linear dependence on the $b^*(\tau), b(\tau)$ -trajectories, the BEC degrees of freedom can be immediately integrated out in the same manner as with the calculation of the generating functional (17).

After eliminating the BEC from (24), for the correlation function $\mathcal{G}_{\mathbf{p}}$ one gets

$$\mathcal{G}_{\mathbf{p}}(t) = \int D[\{a_{\mathbf{q}}^*(\tau)\}, \{a_{\mathbf{q}}(\tau)\}] a_{\mathbf{p}}(t) a_{\mathbf{p}}^*(0) \exp[-iS_P - iS_I]. \quad (25)$$

The above integral is the non-Gaussian functional integral over impurity particle trajectories only, and its non-Gaussian part S_I reads

$$S_I = \int_0^t d\tau \int_0^t d\tau' \sum_{q,q',q''} a_{q'+q}^*(\tau) a_{q'}(\tau) \Gamma_q(\tau - \tau') a_{q''-q}^*(\tau') a_{q''}(\tau'). \quad (26)$$

Here $\Gamma_q(\tau)$ represents the Green's function of the free particle in BEC. Now our aim is to construct the perturbative expansion for the path integral of the form (25) in powers of its non-Gaussian part

$$\mathcal{G}_p^{(n)}(t) = \langle a_p(t) a_p^*(0) \rangle - \langle a_p(t) S_I a_p^*(0) \rangle + \frac{1}{2!} \langle a_p(t) S_I^2 a_p^*(0) \rangle + \dots + \frac{(-1)^n}{n!} \langle a_p(t) S_I^n a_p^*(0) \rangle. \quad (27)$$

The general expression for the n th term of the above expansion reads

$$\begin{aligned} \langle a_p(t) S_I^n a_p^*(0) \rangle &= \sum_{\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_n} \int_0^t d\tau_1 d\tau_2 \dots d\tau_n \\ &\times \int_0^t d\tau'_1 d\tau'_2 \dots d\tau'_n \Gamma_{\mathbf{q}_1}(\tau_1 - \tau'_1) \Gamma_{\mathbf{q}_2}(\tau_2 - \tau'_2) \dots \Gamma_{\mathbf{q}_n}(\tau_n - \tau'_n) \\ &\times \sum_{\mathbf{q}'_1, \mathbf{q}'_2, \dots, \mathbf{q}'_n} \sum_{\mathbf{q}''_1, \mathbf{q}''_2, \dots, \mathbf{q}''_n} \langle a_p(t) a_{\mathbf{q}'_1 + \mathbf{q}_1}^*(\tau_1) a_{\mathbf{q}'_1}(\tau_1) a_{\mathbf{q}''_1 - \mathbf{q}_1}^*(\tau'_1) a_{\mathbf{q}''_1}(\tau'_1) \dots \\ &\times a_{\mathbf{q}_n + \mathbf{q}_n}^*(\tau_n) a_{\mathbf{q}_n}(\tau_n) a_{\mathbf{q}''_n - \mathbf{q}_n}^*(\tau'_n) a_{\mathbf{q}''_n}(\tau'_n) a_p^*(0) \rangle, \end{aligned} \quad (28)$$

where the averaging is performed by the integration over all trajectories with the weight $\exp(-iS_p)$.

First, let us consider the correlation functions of the trajectories $a_q^*(\tau)$ and $a_q(\tau)$ in the integrand of equation (28). Using the general formula (20) together with the expression for the generating functional for the impurity particle in the form of equation (17) where the propagator $G_q(\tau)$ is determined as the Green's function of the free impurity particle, for the correlator of the particle trajectories one gets

$$\begin{aligned} \langle a(t) a^*(\tau_1) a(\tau_1) a^*(\tau'_1) a(\tau'_1) a^*(\tau_2) a(\tau_2) a^*(\tau'_2) a(\tau'_2) \dots a^*(\tau_n) a(\tau_n) a^*(\tau'_n) a(\tau'_n) a^*(0) \rangle \\ = \sum_{P(\{\tau_k\}, \{\tau'_k\})} G(t - P_1) G(P_1 - P_2) \dots G(P_{2n-1} - P_{2n}) G(P_{2n}). \end{aligned} \quad (29)$$

We omitted the momentum indices in the above expression for simplicity. The sum in the right-hand side of equation (29) is performed over all permutation of the time points $\tau_1, \tau_2, \dots, \tau_n, \tau'_1, \tau'_2, \dots, \tau'_n$. This equation which we obtained using the method of generating functional is in fact equivalent to the well-known Wick's theorem. Next, we can substitute equation (29) into expression (28) and do the following: instead of permuting the time points in the correlator (29) we will permute the time points in the product of the BEC propagators $\Gamma(\tau_1 - \tau'_1) \Gamma(\tau_2 - \tau'_2) \dots \Gamma(\tau_n - \tau'_n)$ in the integrand in the right-hand side of equation (28) while the particle correlator has to be taken with the fixed times τ_k, τ'_k , i.e.

$$\begin{aligned} \langle a_p(t) S_I^n a_p^*(0) \rangle &= \int_0^t d\tau_1 d\tau_2 \dots d\tau_n \int_0^t d\tau'_1 d\tau'_2 \dots d\tau'_n \\ &\times \sum_{P(\{\tau_k\}, \{\tau'_k\})} \Gamma(P_1 - P_2) \Gamma(P_2 - P_4) \dots \Gamma(P_{2n-1} - P_{2n}) G(t - \tau_1) G(\tau_1 - \tau'_1) \\ &\times G(\tau'_1 - \tau_2) G(\tau_2 - \tau'_2) \dots G(\tau'_{n-1} - \tau_n) G(\tau_n - \tau'_n) G(\tau'_n). \end{aligned} \quad (30)$$

Now we are able to represent each term of perturbative expansion of the Green's function $\mathcal{G}(t)$ graphically with the help of Feynman's diagrams. Let us represent the product of the

particle propagators by the solid lines connecting the time points

$$G(t - \tau_1)G(\tau_1 - \tau'_1)G(\tau'_1 - \tau_2) \dots G(\tau_n - \tau'_n)G(\tau'_n) = \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \dots \text{---} \bullet \text{---} \bullet \text{---} \quad (31)$$

The number of vertices equals $2n$ where n is the order of perturbation. The right incoming and left outgoing plain lines correspond to the trajectories $a_p^*(0)$ and $a_p(t)$ in the expression for the correlator (29), respectively. Thus the zeroth-order term of expansion is simply given by

$$\mathcal{G}_p^{(0)}(t) = \langle a_p(t)a_p^*(0) \rangle = G_p(t) = \text{---} \quad (32)$$

Then each pair of vertices has to be connected by the BEC propagator Γ by the all possible ways in accordance with the permutation of the time points. We will represent the propagators Γ by wiggly lines. Let us illustrate this technique with the example of the first-order expansion term

$$\mathcal{G}_p^{(1)}(t) = \mathcal{G}_p^{(0)}(t) - \int_0^t d\tau \int_0^t d\tau' \sum_q G_p(t - \tau)G_{p-q}(\tau - \tau')\Gamma_q(\tau - \tau')G_p(\tau) = \text{---} - \text{---} \text{---} \text{---} \quad (33)$$

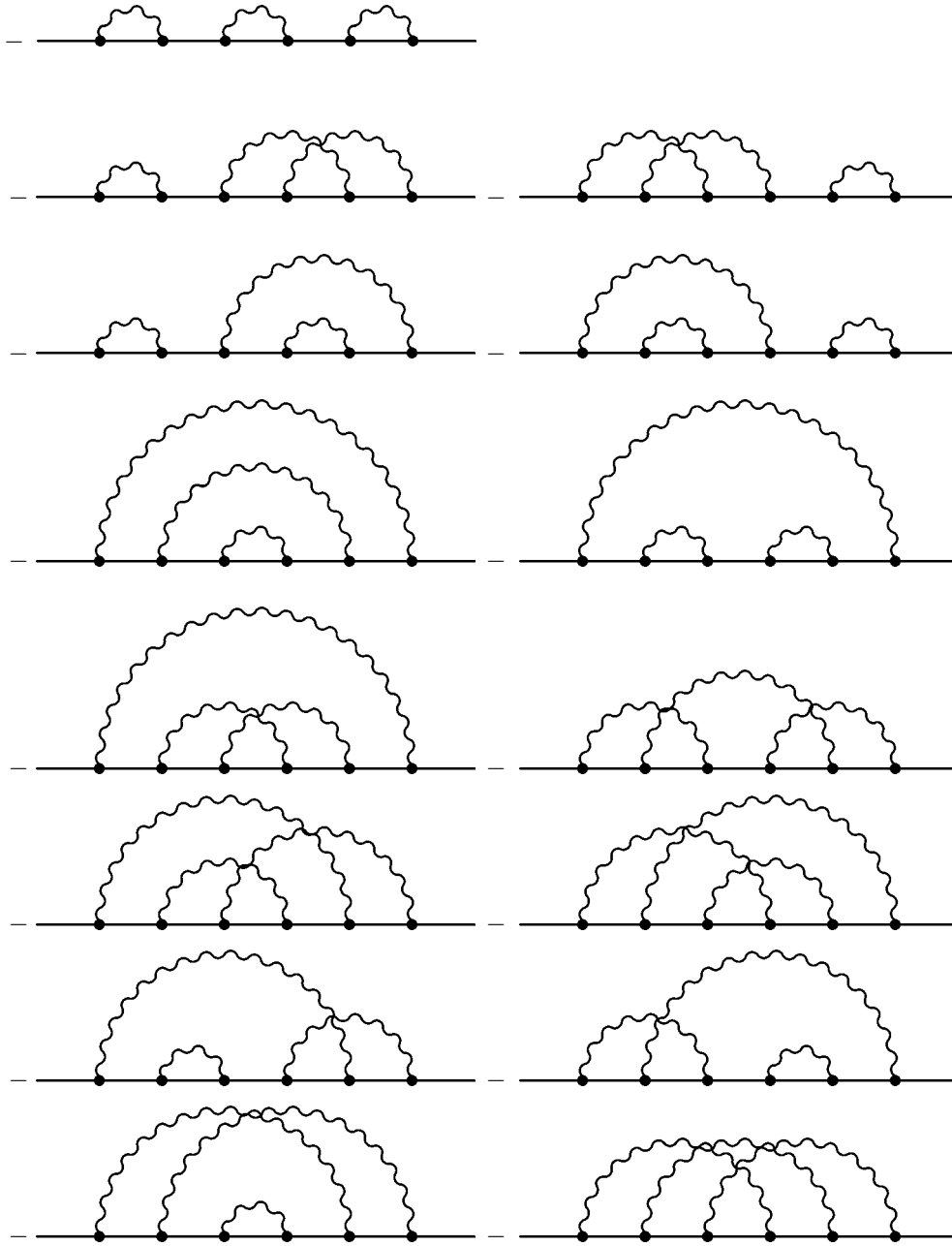
Each propagator line implies the sum over its momentum, while each vertex corresponds to the time point and integration over it. Besides, the vertex insures the momentum conservation rule, i.e. the sum of momenta of all incoming lines equals the sum of momenta of all outgoing lines.

We can connect every pair of vertices in the diagram of n th order by the wiggly Γ -lines by $(2n)!$ different ways because the number of vertices is $2n$. But since only the diagrams with positive direction of time in each propagator $\Gamma(s - s')$, $s > s'$ will bring the non-zero contribution, the whole number of all diagrams L_n of n th order is $L_n = (2n)!/2^n$. On the other hand, we have $L_n = C_2^{2n} C_2^{2n-2} \dots C_2^4$, where $C_k^m = \frac{m!}{k!(m-k)!}$ is the number of all possible choices of pairs of vertices to be connected by the propagator Γ . Next, it is clear that in the sum of n th-order diagrams one can meet identical graphs which can be obtained from each other by permuting the wiggly lines. Thus one can separate all diagrams giving different contribution as $L_n = D_n n!$, where D_n denotes the number of all topologically different graphs, and the factor $n!$ is due to the permutation of every pairs of vertices connected by the wiggly line.

Now let us write down the terms of the second ($D_2 = 3$) and the third ($D_3 = 15$) orders in diagrammatic representation in accordance with the rules established above

$$\mathcal{G}_p^{(2)}(t) = \mathcal{G}_p^{(1)}(t) + \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \text{---} + \text{---} \text{---} \text{---} \text{---} \quad (34)$$

$$\mathcal{G}_p^{(3)}(t) = \mathcal{G}_p^{(2)}(t)$$



(35)

The last step is to separate all irreducible diagrams, i.e. diagrams which cannot be split into two diagrams of lower order by cutting one plain inner line, in all orders of perturbation. Let us define the self-energy graph as the sum of all irreducible blocks of each perturbation

order, i.e.

$$\Sigma_p(\tau - \tau')$$

$$(36)$$

Here the time points τ and τ' in $\Sigma(\tau - \tau')$ denote the left and the right vertices of each irreducible block on the right-hand side of equation, respectively. Then one can rewrite the expansion for the Green's function $\mathcal{G}_p(t)$ with the help of the self-energy part as follows:

$$(37)$$

Each term of perturbation for $\mathcal{G}_p(t)$ is now represented by a convolution of the free propagators G_p and the self-energy part Σ_p , i.e.

$$\begin{aligned}
 \text{---} \circ \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} &= \int_0^t d\tau_1 G_p(t - \tau_1) \int_0^{\tau_1} d\tau_2 \Sigma_p(\tau_1 - \tau_2) \\
 &\times \int_0^{\tau_2} d\tau_3 G_p(\tau_2 - \tau_3) \int_0^{\tau_3} d\tau_4 \Sigma_p(\tau_3 - \tau_4) \dots \int_0^{\tau_{k-1}} d\tau_k \Sigma_p(\tau_{k-1} - \tau_k) G_p(\tau_k).
 \end{aligned} \tag{38}$$

So for the Laplace transform components equation (37) reads

$$\begin{aligned}
 \bar{\mathcal{G}}_p(\omega) &= \bar{G}_p(\omega) + \bar{G}_p(\omega) \bar{\Sigma}_p(\omega) \bar{G}_p(\omega) + \dots + \bar{G}_p(\omega) \bar{\Sigma}_p(\omega) \bar{G}_p(\omega) \dots \bar{\Sigma}_p(\omega) \bar{G}_p(\omega) + \dots \\
 &= \frac{1}{\bar{G}_p^{-1}(\omega) - \bar{\Sigma}_p(\omega)}.
 \end{aligned} \tag{39}$$

Here the bar denotes Laplace transform. Thus at this point we obtained the Dyson's-type equation for the Green's function equation (39). The poles of the Green's function are determined by the solution of the spectral equation $\bar{G}_p^{-1}(\omega) - \bar{\Sigma}_p(\omega) = 0$. The contribution of the self-energy part into the spectral equation can be interpreted as the influence of the cloud of the virtual BEC excitations surrounding the particle. The solution of this equation will be discussed in the following section.

5. The dispersion relation and the energy spectrum of an impurity

In the previous section we obtained the expansion for the self-energy part in powers of coupling constant

$$\Sigma_p(\tau) = \sigma_p^{(1)}(\tau) + \sigma_p^{(2)}(\tau) + \dots, \tag{40}$$

where the n th expansion term $\sigma_p^{(n)}(\tau)$ consists of all diagrams with n wiggly lines in accordance with the expansion (36) and is proportional to g^{2n} . In accordance with equation (39) the Green's function yields

$$\bar{\mathcal{G}}_p(\omega) = \frac{1}{\omega + iE(\mathbf{p}) - \bar{\Sigma}_p(\omega)}, \quad E(\mathbf{p}) = \frac{p^2}{2M}, \tag{41}$$

and its inverse Laplace transform is given by the Fourier–Mellin integral

$$\mathcal{G}_p(t) = \lim_{\varepsilon \rightarrow 0^+} \frac{1}{2\pi i} \int_{-i\infty + \varepsilon}^{i\infty + \varepsilon} \bar{\mathcal{G}}_p(\omega) e^{\omega t} d\omega. \tag{42}$$

Replacing the integration variable in the above integral as $\omega = -i\Omega$, for the origin of the Green's function one gets

$$\mathcal{G}_p(t) = \frac{1}{2\pi i} \int d\Omega \frac{e^{-i\Omega t}}{E(\mathbf{p}) - \Omega + i\bar{\Sigma}_p(\Omega)}, \tag{43}$$

where the integration is performed over the contour shown in figure 1, and $\bar{\Sigma}_p(\Omega) = \bar{\Sigma}_p(\omega = -i\Omega)$. First, let us concentrate on the lowest order perturbative results that can be obtained by taking into account the first expansion term with one loop in the expression for the self-energy part equation (36)

$$\sigma_p^{(1)}(\tau - \tau') = - \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} \text{---} = - \sum_{\mathbf{k}} \gamma_{\mathbf{k}}^2 G_{\mathbf{p}-\mathbf{k}}(\tau - \tau') \Gamma_{\mathbf{k}}(\tau - \tau'). \tag{44}$$

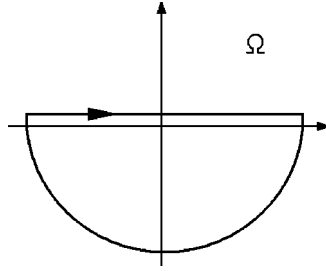


Figure 1. Integration contour for the calculation of inverse Laplace transform of the Green’s function.

Evaluating the Laplace transform of equation (44) and substituting it into equation (39), for the Green’s function in the one loop approximation one gets

$$G_p^{(1)}(t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\Omega \frac{e^{-i\Omega t}}{E(\mathbf{p}) - \Omega + \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{\Omega - E(\mathbf{p}-\mathbf{k}) - \epsilon(\mathbf{k}) + i0} - i0}. \quad (45)$$

The third term in the denominator is significant only if Ω is close to $E(\mathbf{p})$. Thus for the pole of the above integral we have

$$\Omega_0^{(1)} = E(\mathbf{p}) + \sum_{\mathbf{k}} P \frac{\gamma_{\mathbf{k}}^2}{E(\mathbf{p}) - E(\mathbf{p}-\mathbf{k}) - \epsilon(\mathbf{k})} - i\pi \sum_{\mathbf{k}} \delta(E(\mathbf{p}) - E(\mathbf{p}-\mathbf{k}) - \epsilon(\mathbf{k})). \quad (46)$$

As is well known, the real part of the pole of the Green’s function determines the energy spectrum $E_i(\mathbf{p}) = \text{Re}(\Omega)$ while the imaginary part defines the dissipation rate. Thus the second term in the right-hand side of equation (46) represents the correction to the energy of the impurity due to the interaction with BEC while the last term describes the dissipation process, i.e. the energy transfer between impurity and BEC.

Let us calculate the energy of the particle at zero momentum $\mathbf{p} = 0$. After performing the thermodynamic limit ($N \rightarrow \infty, V \rightarrow \infty, N/V = n$), i.e. replacing the sum over momenta $\sum_{\mathbf{k}}$ by the integral $\frac{V}{(2\pi)^3} \int d\mathbf{k}$, the zero-point energy can be written as

$$E_i^{(1)}(p = 0) = gn - \frac{g^2 n}{16\pi^3 m} \int d\mathbf{k} \frac{k^2}{2m\epsilon(k)} \frac{1}{\epsilon(k) + k^2/2m}. \quad (47)$$

In order to prevent the divergence at large momenta in the above integral one has to renormalize the coupling constant g by taking into account the second-order Born approximation for the scattering length a :

$$g = \frac{2\pi a}{m_r} \left(1 + \frac{2a}{\pi} \int dk \right), \quad (48)$$

where $m_r = (1/m + 1/M)^{-1}$ is the reduced mass. The energy reexpanded in powers of the scattering length is now finite and given as

$$E_i^{(1)}(p = 0) = \frac{2\pi an}{m_r} \left(1 + \frac{4amc}{\pi} I_0(m/M) \right), \quad (49)$$

$$I_0(z) = \frac{z\sqrt{z^2 - 1} - \ln(z + \sqrt{z^2 - 1})}{\sqrt{(z^2 - 1)}(z - 1)}. \quad (50)$$

At this point one can consider the interesting case if the impurity has the same mass as the condensate particle and the scattering length a equals the scattering length for the interaction between Bose particles in the condensate, i.e. $c = \sqrt{4\pi an}/m$. Then the energy correction reads ($I_0(z = 1) = 8/3$)

$$E_i^{(1)}(p = 0, m = M) = \frac{4\pi an}{m} \left(1 + \frac{32}{3} \sqrt{\frac{a^3 n}{\pi}} \right) = \mu_B. \quad (51)$$

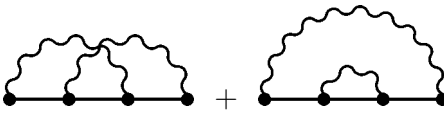
So the energy of the resting impurity in this case coincides with the chemical potential of the interacting Bose gas in Bogoliubov's approximation (the expression for μ_B can be obtained using equation for the ground-state energy of BEC (7) and can be found, for example, in [27]).

The probability for the particle to stay in its initial state $|\mathbf{p}\rangle$ is given by $w_{\mathbf{p}} = |\mathcal{G}_{\mathbf{p}}(t)|^2$ and it decays exponentially like $\exp(-\lambda t)$, where the transition rate λ is given by the imaginary part of the pole $\Omega_0^{(1)}$, i.e.

$$\begin{aligned} \lambda_{\mathbf{p}} &= 2\pi \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \delta(E(\mathbf{p}) - E(\mathbf{p} - \mathbf{k}) - \epsilon(\mathbf{k})) \\ &= \frac{g^2 n}{8\pi^2 m} \int d\mathbf{k} \frac{k^2}{\epsilon(k)} \delta(E(\mathbf{p}) - E(\mathbf{p} - \mathbf{k}) - \epsilon(\mathbf{k})). \end{aligned} \quad (52)$$

The above result corresponds to the Golden rule approximation and reflects the Landau's criterion for the energy dissipation in BEC since the integral in the right-hand side of equation (52) is not zero only if the momentum of the impurity particle p is more than its critical value $p_c = Mc$.

Now we turn to the contribution of the next order perturbation term represented by a couple of two-loop diagrams



$$\begin{aligned} \bar{\sigma}_{\mathbf{p}}^{(2)}(\Omega) &= \sum_{\mathbf{k}, \mathbf{k}'} i\gamma_{\mathbf{k}}^2 \gamma_{\mathbf{k}'}^2 \frac{E(\mathbf{p} - \mathbf{k}) + E(\mathbf{p} - \mathbf{k}') + \epsilon(\mathbf{k}) + \epsilon(\mathbf{k}') - 2\Omega}{(\epsilon(\mathbf{k}) + E(\mathbf{p} - \mathbf{k}) - \Omega - i0)^2 (\epsilon(\mathbf{k}') + E(\mathbf{p} - \mathbf{k}') - \Omega - i0)} \\ &\quad \times \frac{1}{(\epsilon(\mathbf{k}) + \epsilon(\mathbf{k}') + E(\mathbf{p} - \mathbf{k} - \mathbf{k}') - \Omega - i0)}. \end{aligned} \quad (53)$$

The spectral equation defining the poles of the particle Green's function is now given by

$$E(\mathbf{p}) - \Omega_0 + i\bar{\sigma}_{\mathbf{p}}^{(1)}(\Omega_0) + i\bar{\sigma}_{\mathbf{p}}^{(2)}(\Omega_0) = 0. \quad (54)$$

Since the last two terms in the above equation are small, we will find the solution Ω_0 iteratively, i.e. in the form of expansion in powers of coupling constant

$$\Omega_0^{(2)} = E(\mathbf{p}) + i\bar{\sigma}_{\mathbf{p}}^{(1)}(E(\mathbf{p})) - \left. \frac{\partial \bar{\sigma}_{\mathbf{p}}^{(1)}(\Omega)}{\partial \Omega} \right|_{E(\mathbf{p})} \bar{\sigma}_{\mathbf{p}}^{(1)}(E(\mathbf{p})) + i\bar{\sigma}_{\mathbf{p}}^{(2)}(E(\mathbf{p})). \quad (55)$$

The third and the fourth terms in (55) represent the correction of the order g^4 to the result (46). One can see that the imaginary part of the pole coming from the denominator in the right-hand side of equation (53) and defining the correction to the transition rate (52) does not contradict with the Landau's criterion. Finally, the pole with the second-order contribution

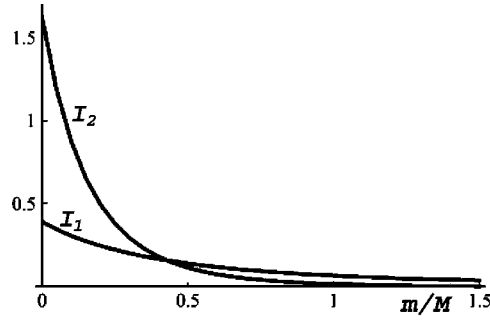


Figure 2. The functions that enter the expression for the effective mass of an impurity in BEC as given by equation (58).

can be written as follows:

$$\begin{aligned} \Omega_0^{(2)}(\mathbf{p}) &= \Omega_0^{(1)} + \frac{g^4 n^2 m^4}{4\pi^6 M} \int d\mathbf{l} d\mathbf{l}' \frac{\mathbf{l}\mathbf{l}'}{\sqrt{(1+4/l^2)(1+4/l'^2)}} \\ &\times \frac{e(l) + e(l') - 2z\mathbf{p}(\mathbf{l} + \mathbf{l}')/k_c}{(e(l) - 2z\mathbf{p}\mathbf{l}/k_c)^2 (e(l') - 2z\mathbf{p}\mathbf{l}'/k_c)^2 (e(l) + e(l') + 2z\mathbf{l}\mathbf{l}' - 2z\mathbf{p}(\mathbf{l} + \mathbf{l}')/k_c)} \\ &+ \text{Im}(\Omega_0^{(2)}(\mathbf{p})). \end{aligned} \quad (56)$$

where $e(l) = l^2(\sqrt{1+4/l^2} + z)$, $k_c = mc$ and $z = m/M$. The integration in the right-hand side of equation (56) is performed over dimensionless vectors \mathbf{l}, \mathbf{l}' . The second-order contribution to the zero-point energy does not depend on the speed of sound and diverges logarithmically at large momenta. It is important to note that the third and higher order corrections to the zero-point energy do not have the divergencies in the momentum integration that are encountered in the first two terms, since the power of momenta in the denominator of the n th order self-energy part is $2(2n - 1)$ while the number of integration variables over momenta space equals n .

Next, we consider the dissipationless motion of the impurity with the momentum p less than the critical momentum Mc , i.e. $\text{Im}(\Omega_0(\mathbf{p})) = 0$, and expand the function $\Omega_0^{(2)}(p)$ up to second order in p . In the absence of anisotropy the term linear in p disappears, and the energy of the impurity can be written in the form

$$E_i^{(2)}(\mathbf{p}) = E_i(\mathbf{p} = 0) + \frac{p^2}{2M_{ef}^{(2)}}, \quad (57)$$

where the effective mass of the impurity is given by following expression:

$$M_{ef}^{(2)} = M \left[1 - \frac{32}{3} g_M I_1 \left(\frac{m}{M} \right) + \frac{8}{3\pi^2} g_M^2 I_2 \left(\frac{m}{M} \right) \right]^{-1}. \quad (58)$$

Here we introduced the new dimensionless expansion parameter

$$g_M = \frac{a^2 n}{p_c} \left(\frac{m}{m_r} \right)^2, \quad p_c = Mc. \quad (59)$$

Two dimensionless functions I_1 and I_2 represent large algebraic expressions that contain the expansion of the integral of equation (56). The evaluation of these functions (numerical for I_2) is shown in figure 2.

The expansion parameter g_M is proportional to $(an^{1/3})^2/a_B n^{1/3}$, where a_B is the scattering length of the particles in BEC, and the parameters $an^{1/3}$ and $a_B n^{1/3}$ are natural dimensionless

small parameters for weakly interacting BEC and weak impurity–BEC coupling, respectively. Thus the value g_M remains small as long as the scattering length a does not exceed the scattering length a_B significantly. The second and the third terms in square brackets in equation (58) represent the correction to the mass of the impurity. Although these corrections are assumed to be small, they show the tendency for increasing the effective mass of the impurity with increasing coupling. As was mentioned in [17], this tendency points out the possibility of self-localization of the impurity particle in BEC.

6. Conclusion

In this work we developed a systematic perturbation theory for the quantum propagator of an impurity in the degenerate BEC. We derived a reduced Bogoliubov-type Hamiltonian for a quantum particle in weakly interacting Bose gas. The perturbation expansion is then built by using the coherent-state path integral formulation for the Green's function of an impurity. The latter allowed us to develop the diagrammatic technique for the calculation of the self-energy part of this system. This technique, i.e. the systematic method for constructing the terms and computation of their weights in the overall expansion for the self-energy is one of the main results of this work.

In this paper, we demonstrate the use of this theory by computing the first two orders of the correction to the free propagator. In this way we obtain the energy spectrum and effective mass of an impurity in BEC to the second order (fourth power of the impurity–BEC coupling parameter). This result may be important in its own right and may be applied directly to the motion of impurities in the weakly coupled Bose condensates. However, we believe that the main significance of this treatment is its capability to approach strongly interacting systems. Among the effects that can be studied using this methodology is the self-localization of an impurity as well as the calculation of dynamical properties of impurities strongly interacting with BEC.

Variational perturbation theory is one of the methods capable of computing properties of strongly coupled systems. The method has been successful in predicting a number of properties of homogeneous BEC [31]. The idea of this method, originally proposed by Feynman and Kleinert [32], is to find an effective weakly coupled potential that gives an accurate estimate of a property in the strongly interacting system. Such potential is found by variation of one of the parameters, for example the mass of impurity, and optimizing its value to achieve the least sensitivity of the property of interest. In other words, one can obtain strong coupling expansions by employing the variational resummation of the ordinary perturbation series [30]. It is known that the first order of the perturbation theory cannot be a good starting point for the variational treatment of the weak coupling expansions. This work gives an access to the higher order corrections of the BEC/impurity system and may be used for such development that can allow the calculation of impurity dynamics in the strongly interacting case.

Finally, we would like to note that in spite of the fact that the diagrammatic expansion developed in this work is applied to the particular problem of an impurity in degenerate BEC, this technique may prove to be more general and can be employed for the wide range of the problems connected with the motion of quantum particle linearly coupled to the environment consisting of non-interacting bosonic modes.

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