Variational approach to the ground state of an impurity in a Bose–Einstein condensate

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Received 10 January 2010, in final form 10 March 2010
Published 26 April 2010
Online at stacks.iop.org/JPhysB/43/105301

Abstract
In this paper, we consider the effect of self-localization of a quantum impurity in a Bose–Einstein condensate. The space correlation function of the impurity is evaluated with the help of the imaginary-time path integral approach. Employing Feynman’s variational method, we calculate the impurity correlation function as well as the energy of the system associated with the impurity. The effect of self-localization predicted before within the Gross–Pitaevskii approach is recovered by our treatment. The strong coupling regime with negative ground state energy is reached by the variational method, and the corresponding correlation function is calculated.

1. Introduction
The theory of atomic-size impurities in Bose–Einstein fluids became a subject of intensive research in the last decade. The theoretical development is largely motivated by recent experiments. The MIT group [1] has studied the dynamics of impurity atoms in the Bose–Einstein condensate (BEC) of ultracold atoms in magnetic traps. Another set of experiments studies the microscopic superfluidity of liquid helium by spectroscopic measurements on molecules embedded in helium droplets [2, 3]. It is generally observed that the microscopic impurity particle interacting with the Bose liquid/gas behaves as a free particle with the effective mass increased by its interaction with the Bose fluid. Such dissipationless quantum motion is observed both for translational motion of particles in the BEC and for rotations of molecules in superfluid helium.

The problem that attracted the attention of theorists was the structure of the ground state of the impurity in the BEC and, in particular, the possibility of the so-called self-localization of an impurity: the appearance of a bound state of an impurity with the BEC despite the purely repulsive interaction potential. Such behaviour has been investigated by a number of authors using linearized Gross–Pitaevskii equations [4–7]. This method allows us to obtain the nonlinear imaginary-time Schrödinger equation for the impurity particle. The energy of the particle becomes negative above a certain value of the coupling strength that depends on the BEC/particle and BEC/BEC interaction potentials. Extension of these results within a fully quantum treatment is an open question and is the major subject of the present work.

In this paper, the matrix element of the reduced density operator of an impurity is calculated allowing the computation of the energy and the space correlation function of the impurity. The system of interest is a particle interacting with a gas of uncoupled Bogoliubov’s excitations. We formulate this matrix element via imaginary-time path integrals. The integral over BEC trajectories is explicitly eliminated and the non-Gaussian functional integral over impurity trajectories needs to be calculated. We treat this integral using the variational approach developed by Feynman for polarons in polar crystals [8]. This method was successfully applied to problems described by the Fröhlich-type Hamiltonian such as polarons, electron–plasmon interaction [9], nucleon–meson interaction [10], many-body fermion problems [11] and many others. Since the Hamiltonian of our model (one particle interacting with uncoupled bosonic modes) is of the Fröhlich type, we believe that such a treatment is successful in our case. We obtain the free energy of an impurity as a function of the coupling constant. The energy increases in the weak-coupling regime in agreement with regular perturbation theory treatments. With a further increase of coupling, it reaches its maximum and then decreases, becoming negative in the...
case of strong coupling. This indicates the existence of a bound state. By computing the correlation function, we obtain the localization radius as a function of the coupling constant. We show that the critical localization radius is of the order of the magnitude of the inverse critical momentum above which the dissipation of particle motion takes place in real-time dynamics.

The Planck constant $\hbar$ and the Boltzmann constant $k_B$ are set to unity throughout the paper.

2. Model Hamiltonian and the statement of a problem

As has been mentioned in section 1, we are going to concentrate on the case of a dilute Bose gas at a temperature much lower than the temperature of condensation. So the gas of weakly interacting Bose particles with mass $m$ can be described as a gas of uncoupled Bogoliubov’s excitations [12, 13], i.e. the Hamiltonian of the BEC has a diagonal form and reads

$$H_B = \sum_k \varepsilon(k) \hat{b}_k^\dagger \hat{b}_k, \quad \varepsilon(k) = \sqrt{\frac{k^2}{2m} - \frac{m^2}{2k^2} c^2}.$$  \hspace{1cm} (1)

Here the bosonic operators $\hat{b}_k^\dagger$ and $\hat{b}_k$ create and annihilate, respectively, the collective excitation with momentum $k$ and with Bogoliubov’s spectrum $\varepsilon(k)$ which has phonon-like behaviour at low momenta, i.e. $\varepsilon(k \to 0) = kc$, where $c$ is the speed of sound.

Next, we consider a quantum particle with mass $M$ interacting with the BEC discussed above. The particle–BEC interaction is described by the term

$$\frac{g}{2V} \sum_{q,k \neq 0} \hat{b}_q^\dagger \hat{b}_q \phi_{q,k} \hat{b}_k$$

where

$$\phi_{q,k} = \sqrt{\frac{Nk^2}{2m\varepsilon}} 
\psi \left( \frac{k^2}{2m} - \frac{m^2}{2k^2} c^2 \right) \sqrt{\frac{N}{2}} 
\square^2 \left( \frac{k^2}{2m} - \frac{m^2}{2k^2} c^2 \right) \frac{N}{2}$$

and $\square$ is the Laplacian operator. The above expression create an annihilation a single particle with momentum $p$. The last term in equation (3) describes the particle–BEC interaction with the coupling constant $g$ depending on the whole number of particles in the Bose gas $N$ in the volume $V = N/n$. The first term in (3) represents the first-order correction to the energy due to the particle–BEC 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 Bogoliubov’s excitations as well as the terms like $\sum_{k,q,k \neq 0} \hat{b}_q^\dagger \hat{b}_q \hat{b}_k \hat{a}_\nu$. This approximation remains valid if the single impurity alters the surrounding BEC only slightly, which is always the case in the macroscopic limit.

In order to describe the statistical properties of the impurity that stays in thermal equilibrium with the BEC environment, we will calculate the space correlation function defined as a matrix element of the reduced density operator

$$C(x, x') = \frac{1}{Z} \langle \{ \hat{b}_k^\dagger(\tau) \hat{b}_k(\tau) \} \rangle$$

Here $\beta$ is the inverse temperature, the Hamiltonian $H$ is defined by equation (3), the trace is performed over all states of the BEC and $Z$ is the partition function. The operator $\psi(z) = \frac{1}{\sqrt{N}} \sum_k \hat{b}_k e^{-ikz}$ annihilates the impurity particle at the point $z$. Due to the momentum conservation in the whole system, the reduced density operator is diagonal in the momentum space. Thus, our task is to calculate the correlation function as the reduced density matrix element between two states of the impurity with the momentum $p$. The above matrix element can be represented as the imaginary-time functional integral [17]

$$C(x - x', \beta) = \frac{1}{Z} \int D[\{ \hat{b}_k^\dagger(\tau) \}, \{ \hat{b}_k(\tau) \}]$$

with the imaginary-time action of the whole system

$$S = \int_0^\beta d\tau \sum_k (\hat{b}_k(\tau) b^\dagger(\tau) + \varepsilon(k) \hat{b}_k(\tau) b^\dagger(\tau))$$

(5)

(6)
The trajectories $b_k/b_k^*$ and $\psi(x)/\psi^*(x)$ correspond to the operators $b_k/b_k^*$ of the BEC and the impurity operators $\Psi(x)/\Psi^*(x)$, respectively. The integration over impurity trajectories in (5) has to be performed with the boundary condition $\psi(x, 0) = \psi^*(x, \beta) = 0$.

First, let us discuss the self-consistent approach to the impurity statistics based on Gross–Pitaevskii-type equations. Because of the linear dependence of the interaction part of the action on the $b_k(\tau), b_k^*(\tau)$ trajectories, the BEC degrees of freedom can be integrated out immediately. After tracing out the BEC, we obtain the functional integral representation of the reduced density matrix of the relevant particle that includes the integration over the particle trajectories only

$$ C(x - x', \beta) = \frac{Z_B}{\beta} \int D[\psi^*(x, \tau)],$$

$$ \{\psi(x, \tau)\} \psi(x', \beta) \psi^*(x, 0) e^{-S_I},$$

(7)

Integral (7) is of non-Gaussian type due to the impurity–BEC coupling, and the action $S_t$ reads

$$ S_t = \int_0^\beta d\tau \int d\tau' \psi^*(x, \tau) \left( \frac{\partial}{\partial \tau} - \frac{\Delta}{2M} \right) \psi(x, \tau)$$

$$ - \int_0^\beta d\tau \int_0^\beta d\tau' \int d\tau'' \psi^*(x, \tau) \psi(x, \tau)$$

$$ \times \Lambda(r - r', \tau - \tau') \psi^*(r', \tau') \psi(r', \tau'),$$

(8)

where the kernel

$$ \Lambda(r - r', \tau - \tau') = \frac{V}{(2\pi)^3} \int dk \, \hat{\gamma}_k^2 \Gamma_k (\tau - \tau') e^{ikr}$$

(9)

depends on the imaginary-time propagator of the free Bose field $\Gamma_k(\tau)$ with the spectrum $\epsilon(k)$:

$$ \Gamma_k(\tau) = (\Theta(\tau) + n_k) e^{-\tau \epsilon(k)}, \quad n_k = \frac{1}{e^{\epsilon(k)/\beta} - 1}.$$  

(10)

Here the function $\Theta(\tau)$ denotes the Heaviside step function, and $Z_B = \prod_k n_k e^{\epsilon(k)}$ is the partition function of free Bogoliubov’s excitations. Having the action of the impurity, one can investigate its classical dynamics described by corresponding Euler’s equations of motion. Varying the action $S_t$ for the impurity wavefunction $\psi_t(x) = \psi(x, \tau) e^{iE}$, one gets the following stationary equation:

$$ E \psi_t(x) + \frac{\Delta}{2M} \psi_t(x) + \frac{\hbar^2 g^2}{\pi}$$

$$ \times \int d\tau' \psi_t(x) \psi^*(x') \psi_t(x') e^{-i\hbar g f(x - x')} = 0.$$  

(11)

Equation (11) describes the particle self-interacting through the screened Coulomb potential. The same equations for the impurity in the weak-coupled BEC can also be obtained directly employing the linearized Gross–Pitaevskii equations with more restricting initial assumptions [5] such as the Hartree approximation for the impurity/BEC wavefunction and using the real-valued BEC wavefunction. In [5], the authors investigated the lowest energy solution of the above equations. They found that equation (11) has the localized solution with negative energy in the strong coupling regime, i.e. when the impurity/BEC interaction is strong enough to compensate for the high kinetic energy of the localized state of the impurity.

Our goal is to describe the effect of self-localization from a purely quantum point of view, i.e. to construct fully a quantum description of the model system employing the path integral formulation of the imaginary-time propagator. For this purpose, let us return to the functional integral for the correlation function with the full impurity-plus-BEC action of the form (5). Our aim is to represent the correlation function as a single Feynman path integral over the impurity trajectories. Let us introduce auxiliary external sources into the action (6) and define the following functional:

$$ F[j^*(r, \tau), j(r, \tau)] = \frac{1}{\beta} \int D[\psi^*(r, \tau), \psi(r, \tau)]$$

$$ \times \exp \left[ - \frac{1}{\beta} \int_0^\beta d\tau' \int \! dr' \psi^*(r, \tau') \hat{K}(r, \tau) \psi(r, \tau)$$

$$ - j(r, \tau) \psi(r, \tau) - j^*(r, \tau) \psi^*(r, \tau) \right],$$

(12)

$$ \hat{K}(r, \tau) = \frac{\partial}{\partial \tau} - \frac{\Delta}{2M} + \sum_k \gamma_k b_k^*(r) e^{ikr} + b_k^*(r) e^{-ikr}$$

(13)

The functional integral on the right-hand side of equation (12) has to be evaluated with the boundary conditions $\psi(r, 0) = \psi^*(r, \beta) = 0$. Since the integral in (12) is Gaussian, it can be evaluated by the stationary phase method. Thus, for the stationary trajectories, one finds

$$ \psi(r, \tau) - \hat{H}(r, \tau) \psi(r, \tau) - j^*(r, \tau) = 0.$$  

(14)

The formal solution of the above equations can be written in the following form:

$$ \psi_t(r, \tau) = \int_0^\tau d\tau' \exp \left( \int_0^\tau \! d\tau' \hat{H}(r, \tau) \right) j^*(r, \tau').$$

(15)

Finally, substituting this solution into the integrand in (12), for the functional $F$, we have

$$ F[j^*(r, \tau), j(r, \tau)] = \exp \left( \int_0^\beta d\tau \int \! dr' \psi_t(r, \tau) \psi_t(r, \tau')$$

$$ \times e^{-\int_0^\tau \! d\tau' \Theta(r - r') \langle j(r, \tau') \rangle} \right).$$

(16)

Now one can see that the correlation function can be written with the help of the generating functional, namely

$$ C(x - x', \beta)$$

$$ = \left\langle \frac{\delta^2}{\delta j(x') \delta j^*(x, 0)} F[j^*(r, \tau), j(r, \tau)] \right\rangle_{j = j^* = 0},$$

(17)

where the averaging is performed as the integration over BEC trajectories with the free action of the BEC as

$$ \langle \cdots \rangle = \frac{1}{Z} \int D[\psi_t^*(\tau), \psi_t(\tau)] \cdots$$

$$ \times \exp \left[ \int_0^\beta d\tau \sum_k \left( b_k^*(\tau) b_k^*(\tau) + \epsilon(k) b_k^*(\tau) b_k(\tau) \right) \right].$$

(18)
Calculating the functional derivative in equation (17) and representing one particle propagator \( \langle j(r, \tau) | e^{-\int_{0}^{\tau} H(r, \tau') ds} | j'(r, \tau') \rangle \) as a Feynman path integral for the correlation function, we have

\[
C(x - x', \beta) = \left\langle \int_{x(0) = x}^{x(\beta) = x'} D[x(\tau)] e^{-ST} \right\rangle.
\]

where the single particle action depends on the coordinate trajectory \( x(\tau) \):

\[
S_p = \int_{0}^{\beta} d\tau \left[ 2 \frac{Mx^2}{2} + \sum_{k} \gamma_k \left( b_k(\tau) e^{ikx(\tau)} + b_k^*(\tau) e^{-ikx(\tau)} \right) \right].
\]

Now we can eliminate the integration over BEC trajectories from equation (19) and get the correlation function as a single Feynman path integral for the impurity

\[
C(x - x', \beta) = \int_{x(0) = x}^{x(\beta) = x'} D[x(\tau)] e^{-SR},
\]

where the impurity action reads

\[
S_R = \int_{0}^{\beta} d\tau \frac{Mx^2}{2} - \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \times \sum_{k} \gamma_k^2 \Gamma_k(\tau - \tau') e^{ik(x(\tau) - x(\tau'))}.
\]

This form of the single particle functional integral is considered in the following section.

3. Feynman’s variational approach

The imaginary-time correlation function in the form of the path integral (21) provides the exact description of the statistics of the impurity surrounded by the degenerate BEC at low temperature. In this section, we calculate this integral approximately using Feynman’s variational approach to the polaron problem [8]. The idea of the original method is to replace the real action of the impurity (22) with the trial action of the form

\[
S_T = \int_{0}^{\beta} d\tau \frac{Mx^2}{2} + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' Q(\tau - \tau') (x(\tau) - x(\tau'))^2,
\]

where

\[
Q(\tau - \tau') = Q_0(\Theta(\tau - \tau') + n_0) e^{-o(\tau - \tau')}, \quad n_0 = \frac{1}{e\omega - 1}.
\]

It is also useful to write the trial action in the extended form as

\[
e^{-S_T} \sim \int D[y(\tau)] e^{-SET},
\]

\[
S_{ET} = \int_{0}^{\beta} d\tau \left[ 2 \frac{Mx^2(t)}{2} + \frac{my^2(\tau)}{2} + \frac{m\omega^2(y(\tau) - x(\tau))^2}{2} \right].
\]

Performing the integration over the trajectories \( y(\tau) \), one recovers the trial action in the form of equation (23) with \( Q_0 = m\omega^3/4 \). Thus, in this variational treatment, we replace the interaction with the original BEC environment by the interaction of a single trial particle with the mass \( m \).

The trial action of the form (23) is assumed to be the zeroth-order contribution, while the difference between real action (22) and trial one has to be considered as a perturbation. Thus, one has to write the following expansion of the correlation function:

\[
C_T(x - x', \beta) = \frac{1 + S_T - S_R}{1 + S_T - S_R},
\]

where we have defined two kinds of averages

\[
\langle \cdots \rangle = \int_{x(0) = x}^{x(\beta) = x'} D[x(\tau)]^{-SR},
\]

\[
\langle \cdots \rangle_0 = \int_{x(0) = 0}^{x(\beta) = 0} D[x(\tau)] \cdots e^{-SR}.
\]

The trial correlation function \( C_T \) in equation (27) still depends on the two variational parameters \( Q_0 \) and \( \omega \) (or \( m \) and \( \omega \)). Thus, in accordance with the principle of minimal sensitivity [18], one has to minimize this expansion with respect to the variational parameters, and the extremum point will give the best variational approximation for the path integral (21). In order to proceed with expansion (27), we have to calculate four functions, namely

\[
\Sigma_1 = \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' Q(\tau - \tau') (x(\tau) - x(\tau'))^2,
\]

\[
\Sigma_2 = \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{k} \Gamma_k(\tau - \tau') \langle \exp[ik(x(\tau) - x(\tau'))] \rangle,
\]

\[
\Sigma_1^0 = \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' Q(\tau - \tau') (x(\tau) - x(\tau'))^2_0,
\]

\[
\Sigma_2^0 = \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{k} \Gamma_k(\tau - \tau') \langle \exp[ik(x(\tau) - x(\tau'))]_0 \rangle.
\]

Expansion (27) in terms of the functions \( \Sigma \) becomes

\[
C_T = \frac{1 + \Sigma_1 + \Sigma_2}{1 + \Sigma_1^0 + \Sigma_2^0}.
\]

In order to calculate the average \( \langle (x(\tau) - x(\tau'))^2 \rangle \) and \( \langle \exp[ik(x(\tau) - x(\tau'))] \rangle \) that enters the functions \( \Sigma_1 \) and \( \Sigma_2 \), respectively, one can use the generating functional of the form

\[
W[j(\tau)] = \int D[y(\tau)] \int_{x(0) = x}^{x(\beta) = x'} D[x(\tau)]
\]

\[
\times \exp \left( -S_{ET} + \int_{0}^{\beta} ds \: j(s) \bar{j}(s) \right).
\]

So the second average \( \langle \exp[ik(x(\tau) - x(\tau'))] \rangle \) can be evaluated by setting \( j(s) = i\hbar(\delta(s - \tau) - \delta(s - \tau')) \), while the first one
is obtained by differentiating the second one twice over $k$ at $k = 0$. The functional integral in (32) can be evaluated by introducing the new variables $q(r) = x(r) - y(r)$ and $r(r) = (M x(r) + m y(r))/(M + m)$. Substituting this replacement into (25), one gets the action $S_{ET}$ in the form

$$S_{ET} = \int_0^\beta d\tau \left[ \frac{(M + m)\dot{r}^2(\tau)}{2} + \frac{\mu q^2(\tau)}{m + M} - j(r) r(\tau) - \frac{\mu}{M} j(r) q(\tau) \right].$$

(33)

$\mu = m M / (m + M)$.

The above action now describes the harmonic oscillator and the free particle in the presence of the external source, and the corresponding functional integral can be easily evaluated. Here, we write down the result of the integration in (32):

$$W[j(r)](x', x) = W_0 \exp \left\{ - (x - x')^2 \left[ \frac{M \mu \tau}{2 M^2} + \frac{\Omega \mu}{2} \coth \Omega \beta \right] \right\}$$

$$+ \int_0^\beta d\tau \left[ \frac{\mu}{2 M} \sinh \Omega \tau + \sinh \Omega (\beta - \tau) \right] \left[ (x' - x) \right]$$

$$+ \int_0^\beta d\tau \int_0^\tau d\tau' \left[ \frac{\tau - \beta - \tau'}{2 \beta M + m} \frac{\mu}{2 M} \right]$$

$$\times \left[ \sinh \Omega (\beta - \tau) - \sinh \Omega \tau + \sinh \Omega (\beta + \tau) + \sinh \Omega \tau - \frac{1}{\sinh \Omega \beta} \right]$$

$$+ \frac{\mu}{4 \Omega M^2} \left[ \frac{\cosh \Omega (\beta/2 | \tau - \tau'|)}{\sinh \Omega \beta} \right].$$

(34)

(35)

where we have introduced the frequency $\Omega = \omega \sqrt{m / \mu}$. The prefactor $W_0$ is the constant coming from the integration over the deviations around the stationary trajectories; hence, it is independent of the end-points $x$ and $x'$. So for the second average $\langle \exp[ik(x(r) - x(r'))] \rangle$, one gets

$$\langle \exp[ik(x(r) - x(r'))] \rangle$$

$$= W_0 \exp \left\{ - (x - x')^2 \left[ \frac{M \mu \tau}{2 M^2} + \frac{\Omega \mu}{2} \coth \Omega \beta \right] \right\}$$

$$+ ik(x' - x) \left[ \frac{\tau - \beta - \tau'}{2 \beta M + m} + \frac{1}{2 \Omega^2} - \frac{\mu}{2 \Omega^2} \sinh \Omega \tau - \sinh \Omega (\beta - \tau) + \sinh \Omega \tau' + \sinh \Omega (\beta + \tau') \right]$$

$$\times \left[ \frac{1}{\sinh \Omega \beta} + \frac{1}{\sinh \Omega \beta} \right]$$

$$- k^2 \left[ \frac{1}{2 M \Omega^2} |\tau - \tau'| \left( \frac{1}{\beta} - \frac{1}{\beta} \right) + \frac{1}{2 \Omega M^2} - \frac{\mu}{2 \Omega M^2} \right]$$

$$\times \left[ \frac{1}{\sinh \Omega \beta} - \cos \Omega (\beta/2 | \tau - \tau'| / \sinh \Omega \beta) \right].$$

(36)

Below, we are always interested in the low temperature limit $\beta \to \infty$. Calculating the first average $\langle (x(r) - x(r'))^2 \rangle$ with the help of the above expression, for the function $\Sigma_1$, one gets

$$\Sigma_1|_{\beta \to \infty} = W_0 \left[ \frac{\Omega^2 + \omega^2}{2 \omega \Omega} (x - x')^2 + \frac{3 \beta}{M \omega \Omega} \right]$$

$$\times \exp \left[ - \frac{\mu \Omega}{4} (x - x')^2 \right].$$

(37)

The calculation of $\Sigma_2$ cannot be done in a closed form and requires some numerical calculations that will be performed in the next sections.

4. Energy of the impurity

In this section, we will investigate the ground state energy of the impurity as a function of the impurity–BEC coupling strength. Let us define the free energy of the system, $E$, as

$$e^{-\beta E} = \int_{(x(\tau))=0}^{(x(\beta))=0} D[x(\tau)] e^{-S_T} = (e^{S_T - S_0})_0.$$

(38)

In the zero temperature limit, free energy coincides with the ordinary energy and shows the difference between the coupled and uncoupled impurity/BEC system.

Expression (38) up to first cumulant reads

$$e^{-\beta E_0(\Omega, \omega)} = (1)_0 \exp \left\{ \frac{(S_T - S_0)}{(1)_0} \right\},$$

$$E(\Omega, \omega) = E_0 + E_1 + E_2.$$

The zero energy contribution $E_0$ is

$$e^{-\beta E_0} = \int_{(x(\tau))=0}^{(x(\beta))=0} D[x(\tau)] e^{-S_T - W_0} = W_0,$$

(40)

and the first-order contribution terms are defined as

$$E_1 = - \frac{1}{\beta W_0} \Sigma^0_1, \quad E_2 = - \frac{1}{\beta W_0} \Sigma^0_2,$$

(41)

where $\Sigma^0_{1,2}$ is defined by equation (30). While the terms $E_1$ and $E_2$ can be evaluated directly employing the generating functional, the first term $E_0$ cannot be calculated explicitly using formula (40). In order to find $E_0$, one has to note that

$$\int_0^\beta d\tau \int_0^\beta d\tau' Q(\tau - \tau')(x(\tau) - x(\tau'))^2_0 = -m \frac{d}{dm} e^{-\beta E_0}.$$

(42)

Using the result (37), we can get the following equation for zero-order energy:

$$\frac{dE_0}{dm} = \frac{3}{4 \Omega \Omega} \omega^2, \quad E_0(m = 0) = 0.$$

(43)

The solution of the above equation is

$$E_0 = \frac{3}{2} (\Omega - \omega), \quad E_0 + E_1 = \frac{3}{4} (\Omega - \omega)^2.$$
Now the calculation of the contribution $E_2$ is left. Using formula (36), in the zero temperature limit, one can give the following expression for $E_2$:

$$E_2 = -\int_0^\infty \text{d} \tau \sum_k \gamma_k^2 \exp\left[-\epsilon(k) \tau - \frac{k^2}{2}\right] \times \left(\frac{\alpha^2 \tau}{\Omega^2 M} + \frac{\Omega^2 - \omega^2}{\Omega^2 - M \Omega}\right).$$

(45)

First, let us consider the weak coupling limit, i.e. $Q_0 \to 0$ or $m \to 0$, so that $\Omega \sim \omega$. Thus, we have in the lowest order $E_0 + E_1 = 0$, and the energy $E$ is given by the first expansion term of the ordinary perturbation theory:

$$E^{\text{weak}} = E_2^{\text{weak}} = -\sum_k \gamma_k \frac{1}{\epsilon(k) + \frac{\Omega^2}{\Omega^2}}.$$  

(46)

In order to prevent ultraviolet divergence in the above sum over momenta, one has to renormalize the coupling constant $g$ according to the second-order Born approximation. For this purpose, we must add the zero-order energy term $g$ over momenta, one has to renormalize the coupling constant $g$ in powers of scattering length $a$ for the impurity–BEC interaction:

$$g = \frac{2\pi a}{m} \left(1 + \frac{2a}{\pi} \int \text{d} k\right), \quad m_r = \frac{m_B M}{m_B + M}. \quad (47)$$

The weak coupling energy re-expanded in powers of scattering length is now finite and reads

$$E^{\text{weak}} = m_B c^2 \alpha (1 + z) \int_0^\infty \text{d} l \left[1 - \frac{1 + z}{\sqrt{1 + 4/l^2}(\sqrt{1 + 4/l^2) + z}}\right].$$

(48)

Here we have introduced the dimensionless coupling parameter $\alpha = 4a \pi/(m_B c)$ and the mass ratio $z = m_B / M$. Below we always use the renormalized expression for $E_2$ which is

$$E^{\text{en}}_2 = E_2 + \frac{4a^2 \pi}{m_r} \int \text{d} k.$$  

(49)

Finally, the whole expression for the ground state energy can be written in the integral form

$$E^{\text{en}}(\Omega, \omega) = \frac{3}{4} \left(\frac{\Omega - \omega^2}{\Omega}\right) + \alpha (1 + z) \int_0^\infty \text{d} l \left[1 - \frac{1 + z}{2 \sqrt{1 + 4/l^2}}\right] \times \int_0^\infty \text{d} s \exp\left(-\frac{l^2 \sigma(s)}{2}\right),$$

(50)

where

$$\sigma(s) = s \sqrt{1 + 4/l^2} + sz \frac{\omega^2}{\Omega^2} + \frac{\Omega^2 - \omega^2}{\Omega^2}(1 - e^{-\Omega s}),$$

(51)

The integration in (50) is performed over the dimensionless variables $s$ and $l$, and the energy $E(\Omega, \omega)$ as well as the frequencies $\Omega$ and $\omega$ are now measured in the units $m_B c^2$.

5. Impurity correlation function

Now let us directly consider the correlation function $C(x)$. Using the expression for the function $\Sigma_1$, equation (37), one can rewrite expansion (27) up to first cumulant as

$$C_T(x, \beta \to \infty) = \exp\left[\beta E_2 - \frac{M \Omega}{8} \left(\frac{\Omega^2 - \omega^2}{\Omega^2}\right)^2 x^2 + \frac{\Sigma_2(x)}{W_0(x)}\right].$$

(52)
The correlation function can be written down in the integral form:

\[
C_T(x, \beta \to \infty) = \exp\left\{-\frac{z\Omega}{8} \left(\frac{\Omega^2 - \omega^2}{\Omega^2}\right)^2 x^2\right\} + \alpha \left(\frac{1}{2}\right) \int_0^\infty dl \int_0^\beta ds \int_0^\infty ds' \int_0^{\beta'} ds'' \frac{l^2}{\sqrt{1 + 4/l^2}} \exp\left(-\frac{l^2\sigma_1(s-s')}{2}\right) \left(\frac{\sin(lx\sigma_2(s-s'))}{lx\sigma_2(s-s')} - 1\right),
\]

(53)

where the function \(\sigma_1(s-s')\) is defined by equation (51) and

\[
\sigma_2(s-s') = \frac{\omega^2}{\Omega^2} \frac{s-s'}{\beta''} + \frac{1}{2} \frac{\Omega^2 - \omega^2}{\Omega^2} \frac{1}{\sinh \Omega \beta'}
\times (\sinh \Omega s - \sinh \Omega (\beta - s) - \sinh \Omega s' + \sinh \Omega (\beta - s')).
\]

(54)

As in equation (50), the integration on the right-hand side of equation (53) is performed over the dimensionless variables \(s, s'\) and \(l\). The temperature \(1/\beta\) and the frequencies \(\Omega\) and \(\omega\) are measured in units \(m_Bc^2\), while the variable \(x\) is defined in units \(1/m_Bc\). Finally, in order to find the best approximation for the correlation function, expansion (53) has to be optimized with respect to the pair of variational parameters \(\Omega, \omega\). In general, if the optimization procedure is directly applied to the expansion for the correlation function, the optimized values of variational parameters should depend on the coordinate \(x\). However, it turns out that instead of the variational optimization of the coordinate-dependent correlation function, one can use the optimal values of the variational parameters obtained from the optimization of energy. These coordinate-independent values then have to be substituted into the expansion for the correlation function giving the variationally improved result, i.e. convergent strong coupling expansion for the correlation function. This scheme of the variational perturbation theory was successfully applied for the variational solutions of time-dependent equations in nonlinear dynamics [19, 20].

We will also define the mean value of \(x^2\) representing the square of the radius of localization or polaron radius as

\[
\langle x^2 \rangle = \frac{\int x^2 C(x) dx}{\int C(x) dx}.
\]

(55)

Figure 4 shows the mean square of the radius of localization as a function of coupling constant. It has an inverse dependence on the coupling strength. The inset shows the correlation function itself for different values of the coupling strength. The correlation function has a Gaussian-like shape regardless of \(\alpha\) which means that formally the particle is always localized. This is the consequence of the choice of the trial action used in this method. However, this correlation function should converge to the true one at large values of the interaction strength. It is interesting to examine the localization radius at the coupling constant \(\alpha_e\) at which the energy has maximum, i.e. \(dE(\alpha)/d\alpha|_{\alpha_e} = 0\). We note that \(\langle x^2(\alpha_e) \rangle \sim 1/m_Bc\).

This can be expressed through a so-called healing length of the BEC \(\xi = 1/cp_c\), where \(p_c = Mc\) is the critical momentum of the impurity above which the dissipation takes place in case of real-time dynamics in accordance with Landau’s criterion. This leads to \(\sqrt{\langle x^2(\alpha_e) \rangle} \sim 1/p_c\), or using the Heisenberg uncertainty for the localized particle \(\sqrt{(p^2)} \sim p_c\), i.e. the average momentum of a particle at the point of self-localization.

**Figure 2.** Energy optimized with respect to \(\Omega\) as a function of the coupling constant \(\alpha\) for different values of the second variational parameter \(\omega\).

**Figure 3.** Critical value of the coupling constant \(\alpha_c\) as a function of the mass ratio \(m_B/M\).

**Figure 4.** Mean value of \(x^2\) as a function of the coupling constant, \(x\) is shown in units \(1/m_Bc\). Inset: the correlation function \(c(x)\) for different values of the coupling constant, \(\alpha = 0.5\) (upper curve), \(\alpha = 1, 5\) and \(\alpha = 10\) (lower curve).
is of the order of the critical momentum $p_c$. One can make physical sense of this fact by noting that the tendency of self-localization appears when the exchange of energy between the particle and the BEC becomes possible.

### 6. Conclusion

In this work, we considered a problem of the self-localization of an impurity in a degenerate BEC. This problem has been considered previously using the mean-field approach. Here we used a full quantum description of the ground state of the impurity surrounded by the BEC. The variational perturbation method was employed to calculate the imaginary-time propagator of impurity in the degenerate BEC. The free energy and the spatial correlation of the impurity in the BEC were obtained as a function of the coupling strength. Our results point to a possible relation between self-localization and real-time particle/BEC energy exchange. In this work, we explicitly used the degeneracy of the BEC. However, the methodology developed in this paper can be extended to Bose systems without the assumption of diluteness. The latter can be done by using the four-point Green’s function of the strong coupled Bose liquid [21] in the leading expansion term instead of the degenerate BEC propagator used in this work.

**Acknowledgment**

This work has been supported by the NSF CAREER award ID 0645340.

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