Functional Integration in Bose Systems with Hard-Core Interaction

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Abstract

A grand canonical ensemble of interacting bosons is considered. The zero temperature phase diagram is evaluated from the mean-field approximation of the functional integral. Three phases are found: a superfluid, a normal fluid and a Mott insulator.

Quantum systems with many-body interactions are an important application of functional integrals. As an example a model of interacting bosons is considered. It is defined by the Hamiltonian

\[ H = \sum_{<r,r'>} J_{r,r'} \Phi_r^\dagger \Phi_{r'} - \mu \sum_r \Phi_r^\dagger \Phi_r + \frac{V}{2} \sum_r \Phi_r^\dagger \Phi_{r'}^\dagger \Phi_{r'} \Phi_r, \tag{1} \]

where \( \Phi_r^\dagger \) (\( \Phi_r \)) creates (annihilates) a boson at the lattice site \( r \). The first term describes bosons hopping from site \( r' \) to a nearest neighbor site \( r \). \( \mu \) is a single particle potential and \( V \) the coupling constant of an on-site interaction.

Following the standard procedure (e.g. Ref.\[1\]) the corresponding functional integral for a grand canonical ensemble of bosons reads

\[ Z = \int \exp(-S) \mathcal{D}[\phi, \phi^*] \tag{2} \]

with the action

\[ S = \Delta \sum_{r,t} \frac{1}{\Delta} \phi^*(r,t)[\phi(r,t) - \phi(r,t - \Delta)] + \Delta \sum_t \frac{1}{\hbar} H[\phi^*(r,t), \phi(r,t - \Delta)]. \tag{3} \]

We have introduced a discrete imaginary time with interval length \( \Delta \) and a complex field \( \phi \) with periodic boundaries in time \( \phi(t = 0, r) = \phi(t = \beta \hbar, r) \). The parameter \( \mu \) plays in (2) the role of the chemical potential.

The local part of the Hamiltonian in \( S \) can be approximated \( \phi^*(r,t)\phi(r,t - \Delta) \approx \phi(r,t)\phi^*(r,t) = |\phi(r,t)|^2 \), neglecting terms of \( O(\Delta^2) \) in \( S \). [1] The interaction term
has a positive coupling constant $V$ (repulsion). Thermal fluctuations are switched off by taking implicitly the limit $\beta \to \infty$. A random path expansion \cite{3} can be created by extracting the local part from the action

$$S_0 = -\Delta \sum_x \left[ (\mu - 1/\Delta) n_x - \frac{V}{2} n_x^2 \right], \quad (4)$$

where $n_x = |\phi_x|^2$ and $\hbar = 1$. The expansion in terms of $S_1 \equiv S - S_0$ generates locally powers of the complex field $\phi_x$ and $\phi_x^*$. Since $S_0$ does not depend on the phase of $\phi_x$ we obtain from the integration w.r.t. $\phi$ nonzero quantities only if $\phi_x$ and $\phi_x^*$ appear with the same power at each point $x = (t, r)$

$$\int \phi_x^{l_2} \phi_x^{* l_2} \exp \left\{ \Delta [(\mu - 1/\Delta) n_x - \frac{V}{2} n_x^2] \right\} d\phi_x^* d\phi_x = g_l \delta_{l_l l_2}. \quad (5)$$

Thus, the random path expansion of the partition function leads to a grand-canonical ensemble of Bose world lines (BWLS), going from $t = 0$ to $t = \beta$, which are directed along the $t$-axis. The interaction of the bosons corresponds to the coefficient $g_l$ at $x$ which counts $l$ visiting bosons at $r$ at the time $t$. The statistics of the BWLS simplifies essentially if we apply a hard-core approximation by introducing the restriction that a point $x$ can be visited at most by one boson

$$g_l = 0 \quad \text{for} \ l \geq 2. \quad (6)$$

This condition projects onto boson realizations with hard-core interaction at each point. The contributions to the expansion are empty points with weight $g_0 \equiv \zeta$ and world line elements which connect points $x$ and $x'$ with statistical weight

$$w_{x,x'} \equiv w_{x'-x} = \begin{cases} \Delta g_1 J_{r,r'} \equiv \alpha & \text{for } x' = x + e_{\mu}' \\ \frac{1}{\Delta} & \text{for } x' = x + \Delta e_t \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

e_{\mu}'$ are the unit vectors in the $d$-dimensional space, $e_t$ is the unit vector in time and $e_{\mu}' = e_{\mu} + \Delta e_t$. This model has only two independent parameters, $\alpha$ and $\zeta$. We may write for the partition function of a system on a lattice with $N$ sites

$$Z_{h,-c} = \sum_{n=0}^{N} \frac{\zeta^{(N-n)} \beta}{n!} \sum_{\{r_j(t)\}_{n} \in I_n} P(\{r_j(t)\}_{n}), \quad (8)$$

where $P(\{r_j(t)\}_{n})$ is the weight of a given configuration $\{r_j(t)\}_{n}$ of $n$ BWLS

$$P(\{r_j(t)\}_{n}) = \prod_{x,x' \in \{r_j(t)\}_{n}} w_{x,x'}. \quad (9)$$

$I_n$ are all configurations of BWLS going from $t = 0$ to $t = \beta$ which are allowed by the hard-core condition. It has been shown that the partition function of hard-core bosons \cite{8} can be rewritten for dimensions $d > 1$ in terms of interacting fermions \cite{3, 4, 5, 6}

$$S_{\text{form}} = \sum_{x,x'} (w_{x,x'} + \zeta \delta_{x,x'} \bar{\psi}_x \psi_{x'} \bar{\psi}_{x'} \psi_x), \quad (10)$$

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with Grassmann fields $\psi^a_x$. The hard-core interaction is now represented by the exclusion (Pauli) principle of the fermions. Especially in $d = 1$, the hard-core bosons cannot exchange their positions. This implies that an additional interaction between the fermions is not necessary, and the hard-core bosons are equivalent to non-interacting fermions [6].

The hard-core boson model has been generalized to a model of bosons with $N$ colors [4] or a model with $N$ levels at each point [5]. In the latter the bosons can occupy the $N$ levels statistically. In both cases the limit $N \to \infty$ can be solved exactly.

The formal reason is a formation of composite fields from pairs of fermions. For the $N$ color bosons these are nonlocal fields and in the case of the $N$ bosonic levels these are local fields. The composite fields do not depend on the number $N$ but $N$ appears as a prefactor of the action. Therefore, a saddle point integration can be performed for $N \to \infty$ in both cases. The results of the calculations of Refs. [4, 5] will be used in the following to derive the phase diagram of hard-core bosons at zero temperature.

a) local order parameter: Superfluid (SF)

The effective functional integral of the $N$ level model of Ref. [5] is related to a local complex order parameter field $(\varphi_x, \chi_x)$. The corresponding partition function reads

$$Z_{\text{loc}} = \int \exp \left\{ -N \left[ (\varphi, v_1^{-1} \varphi^*) + (\chi, \chi^*) - \sum_x \log[\zeta + (\varphi_x + i\chi_x)(\varphi_x^* + i\chi_x^*)] \right] \right\} \mathcal{D}[\varphi, \chi],$$

(11)

where $v_1$ is the matrix $w + 1$. There are two mean-field solutions for the saddle point equation $\delta s_{\text{loc}} = 0$: a trivial one with $\varphi = \chi = 0$ and a nontrivial one with $\varphi = -i\chi = 2\sqrt{1 - \zeta}$. The stability of the two solutions is found from the fluctuations around the saddle point [5]: the trivial solution is stable for $\zeta > \alpha^4$ and the nontrivial one for $0 \leq \zeta \leq \alpha^4$. Thus the critical point is $\zeta_c = \alpha^4$. The mean-field approximation of the action is $-\log \zeta$ for the trivial solution and $\alpha^2 - 4 \log \alpha - \zeta/\alpha^2$ for the nontrivial solution. The fluctuations are gapless for $0 \leq \zeta \leq \alpha^4$ due to Goldstone bosons created by a spontaneously broken $U(1)$ symmetry. The corresponding phase is a superfluid. This result can also be obtained if a Ginzburg-Landau expansion is applied directly to the action in (11). The expansion should be valid for small density of bosons. This is very similar to the discussion of weakly interacting bosons [7]. However, this mean-field solution is not a complete description of the physical states of hard-core bosons on a lattice if higher densities are included. This can be seen if a nonlocal order parameter is considered.

b) nonlocal order parameter: Normal Fluid (NF) and Mott Insulator (MI)

It is possible to relate an order parameter field to the elements of the BWLs by replacing $w_{x,x'} \to u_{x,x'}$ [3, 4]. The partition function then reads

$$Z_{\text{nonloc}} = \int \exp \left\{ -N \sum_{x,x'} \frac{(u_{x,x'})^2}{w_{x,x'}} + 2N \log \det(\sqrt{\zeta} + u) \right\} \mathcal{D}[u].$$

(12)

Two different contributions can be distinguished, one is the longitudinal component
$u_{x,x+\Delta x_t}$ and the other the transverse component $u_{x,x+e'_{\mu}}$. A mean-field approximation $u_{x,x+\Delta x_t} \approx \sigma_\parallel$ and $u_{x,x+e'_{\mu}} \approx \sigma_\perp$ has to satisfy the saddle point conditions

$$\frac{\partial s_0}{\partial \sigma_\parallel} = \sigma_\parallel - \frac{2}{\sigma_\parallel} I = 0, \quad \frac{\partial s_0}{\partial \sigma_\perp} = 2d\sigma_\perp - \frac{2}{\sigma_\perp} (n - I) = 0$$

with the integrals $I = \sigma_\parallel \int_{-1}^{1} \Theta(\kappa'^2 - \zeta) / k d' \rho(\kappa) d\kappa$ and $n = \int_{-1}^{1} \Theta(\kappa'^2 - \zeta) \rho(\kappa) d\kappa$. $n$ is the density of BWLs, $\kappa' = 2d\sigma_\perp \kappa + \sigma_\parallel$ and $\rho(\kappa) = \int \delta[(1/d) \sum_{j=1}^{d} \cos k_j - \kappa] d k_1 \ldots d k_d / (2\pi)^d$. $\Theta$ is the Heaviside step function. The mean-field action reads

$$s_0 = d\sigma_\perp^2 + \frac{1}{2} \sigma_\parallel^2 - \log \zeta - \int_{-1}^{1} \log(\kappa'^2 / \zeta) \Theta(\kappa'^2 - \zeta) \rho(\kappa) d\kappa - i\pi.$$  

The saddle point conditions (13) imply $\sigma_\parallel^2 + 2d\sigma_\perp^2 = 2n$. There are three different solutions: $(\sigma_\parallel, \sigma_\perp) = (0, 0)$ (empty phase), $(0, \sqrt{n/d})$ (NF) and $(\sqrt{2n}, 0)$ (MI). The approximation $\rho(\kappa) \approx (1/2) \Theta(1 - |\kappa|)$ gives for the mean-field action the values shown in Table 1, where $\zeta = 4d(1-n)^2 \alpha^2$ for the NF. Although the SF of a) is also a phase with fluctuating BWLs, the NF can be distinguished by the fact that its fluctuations have a gap in contrast to the gapless fluctuations of the SF. Moreover, the SF has a nonzero winding number in contrast to the zero winding number of the NF. The fluctuations of the MI also have a gap which is related to an incompressible array of BWLs. The latter is commensurate with the lattice. An additional nonlocal interaction leads to many commensurate MI phases [6].

**Discussion:** For large values of $\zeta$ and $T = 0$ there will be always an empty phase (i.e., no bosons). (In the case of nonzero temperatures this phase would be a NF due to thermal fluctuations.) The parameter $\alpha$ is the hopping rate of the bosons. Starting from the empty phase at zero temperature the density can be increased by a reduction of $\zeta$. Depending on the values of $\alpha$ the NF (small $\alpha$) or the SF (large $\alpha$) will be reached. An increasing density will eventually destroy the SF due to strong collisions between the bosons, and a transition to a NF will take place. Finally, even the NF will be destroyed: a state can be formed which is commensurate with the lattice, provided $\alpha$ is not too large. This is the MI. As an examples the phase diagram is shown for $d = 3$ in Fig.1.

| Table 1: The mean-field solutions for local and nonlocal order parameters |
|---------------------------------------------------------------|
| phase: Empty Phase   | Fluid Phase   | Mott Insulator |
| density: $n = 0$    | $0 < n < 1$  | $n = 1$          |
| $\sigma_\parallel$: 0   | 0            | $\sqrt{2n}$    |
| $\sigma_\perp$: $\sqrt{n/d}$  | 0            | 0               |
| $s_{\text{nonloc}}$: $-\log \zeta$ | $3n - \log n - 2 \log(2\sqrt{d} \alpha)$ (NF) | $1 - \log 2$          |
| $\varphi$: 0         | $2\sqrt{1 - \zeta/\alpha^2}$ | $\alpha^2 - \zeta/\alpha^2 - 4 \log \alpha$ (SF) |
| $s_{\text{loc}}$: $-\log \zeta$ | $\alpha^2 - \zeta/\alpha^2 - 4 \log \alpha$ (SF) | $-$            |
Fig1: $T = 0$ phase diagram for hard-core bosons. $\alpha$ is the hopping rate of the bosons and $\sqrt{\zeta}$ the fugacity of empty sites. Thermal fluctuations ($T > 0$) would destroy the empty phase and change it into a NF.

References

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