Fluctuating Paths and Fields, Eds. W. Janke, A. Pelster, H.-J. Schmidt, and M. Bachmann
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NOTE ON THE PATH-INTEGRAL VARIATIONAL APPROACH IN MANY-BODY THEORY

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I discuss how a variational approach can be extended to systems of identical particles (in particular fermions) within the path-integral treatment. The applicability of the many-body variational principle for path integrals is illustrated for different model systems and is shown to depend crucially on whether or not a model system possesses the proper symmetry with respect to permutations of identical particles.

1 Introduction

In the path-integral formulation of quantum mechanics, the so-called *Jensen-Feynman inequality* provides an upper bound to the free energy of a quantum system, if properly applied. It was introduced [1] in Feynman's path-integral approach to the Fröhlich polaron (see formula (8.40) in Ref. [2]):

$$F \leq F_M + \frac{1}{\beta}\langle S - S_M \rangle_{S_M} \text{ if } S, S_M \text{ are real.} \tag{1}$$

In the variational functional, F and S are the free energy and the action functional[a] of the system under consideration, whereas F_M and S_M are the free energy and the action functional of a model system; the temperature is described by the parameter $\beta = 1/k_B T$. Angular brackets mean a weighted

[a] It is implicitly assumed that the action functional and the path integral are expressed in the imaginary-time variable. This convention is followed throughout the present paper.

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average over the paths [2]:

$$\langle \bullet \rangle_{S_M} \equiv \frac{\int \bullet \exp(-S_M) D(\text{path})}{\int \exp(-S_M) D(\text{path})}. \tag{2}$$

A rigorous argument to prove the inequality (1) is based on the convex nature of the exponential $\exp(x)$ of a *real* stochastic variable x (see e.g. Fig. 11-1 in Ref. [3]), which leads to $\langle e^x \rangle \geq e^{\langle x \rangle}$ with $\langle x \rangle$ being the weighted average of x.

Apart from Feynman's variational treatment of the ground-state energy of a polaron, the path-integral approach based on the Jensen-Feynman inequality was successfully applied to a series of problems [5], e.g. to the calculation of the effective classical partition function [4,6] and of quantum corrections to the free energy of nonlinear systems [7,8], to the description of all critical exponents observable in second-order phase transitions [9], and to the problem of bipolaron stability [10,11].

The derivation of the Jensen-Feynman inequality crucially depends on the assumption that both the action and the trial action are *real* functionals. As already recognized by Feynman (see Ref. [3], p. 308), its application to a *polaron in a magnetic field* therefore becomes problematic, because the action functional S for a polaron in a magnetic field (and any reasonable trial action S_M) is no longer real-valued. A discussion of this problem lies beyond the scope of the present paper. For more details on the status of this problem, see the literature [12–18].

The Jensen-Feynman inequality is reminiscent of the Bogoliubov inequality [19,20], which provides the following upper bound to the free energy F of a system described by the Hamiltonian H

$$F \leq F_M - \frac{1}{\beta} \frac{\mathrm{Tr}\left[(H - H_M)\, e^{-\beta H_M} \right]}{\mathrm{Tr}\left(e^{-\beta H_M} \right)} \text{ if } H, H_M \text{ are Hermitian,} \tag{3}$$

where H_M is the Hamiltonian of some trial system with free energy F_M. The Rayleigh-Ritz variational principle (see e.g. Ref. [21], p. 172) for the ground-state energy $E \leq \langle \Psi_M | H | \Psi_M \rangle / \langle \Psi_M | \Psi_M \rangle$ with a trial state $|\Psi_M\rangle$ is the zero-temperature limit of the Bogoliubov inequality.

The condition that S and S_M are real in (1) is not necessarily equivalent to the requirement that H and H_M are Hermitian in (3). If the Hamiltonians H and H_M in the Bogoliubov inequality are Hermitian operators corresponding to Lagrangians L and L_M in the Jensen-Feynman inequality, then the one-to-one correspondence between (1) and (3) guarantees the validity of the

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Jensen-Feynman inequality, even if the action functionals are not real (e.g. for a particle in a magnetic field).

However, both inequalities do not necessarily have the same physical content: for a system with action S it is not always possible to derive a corresponding Hamiltonian. For example, for the Fröhlich polaron (in the absence of a magnetic field) the strength of the Jensen-Feynman inequality lies in the fact that it remains valid after the elimination of the phonons, with a *retarded* effective action functional, for which no corresponding Hamiltonian representation is known. In the operator formulation, the phonon elimination can formally be realized with ordered-operator calculus, but this approach involves *non-Hermitian* effective operators in the electron variables.

Fermion systems (with parallel spins) form an important class of systems for which the Jensen-Feynman inequality is not directly applicable (whereas the Bogoliubov inequality remains valid in the Hilbert space of antisymmetric states under permutations of the particle coordinates). The reason is that the path integral for *fermions* with parallel spin, *if expressed in the full coordinate space*, is a superposition of path integrals with all possible permutations of the particle coordinates, with negative signs for all odd permutations. For *bosons*, no negative signs result from the permutations, and the application of the Jensen-Feynman inequality presents no problems. Therefore, only the many-fermion problem will be explicitly addressed below.

2 Path Integral Approach for Many-Body Systems

Recent studies on the path-integral approach to the many-body problem for a fixed number of *identical particles* by Brosens, Lemmens and Devreese [22] have allowed to calculate the Feynman-Kac functional on a state space for N indistinguishable particles, which was found by imposing an ordering on the configuration space, and the introduction of a set of boundary conditions in this state space. The path integral (in the imaginary-time variable) for identical particles was shown to be positive within this state space. This implies (see subsection 3.1 for more details) that a many-body extension of the Jensen-Feynman inequality was found, which can be used to evaluate the partition function for interacting identical particles (Ref. [22], p. 4476, reference [48]). This many-body variational principle for path integrals was applied to the study of thermodynamical properties of a spin-polarized gas of bosons (Ref. [24], abstract, Eq. (3); Ref. [25], Eq. (13)). The applicability of the variational principle as formulated in Ref. [22] for many-body problems

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was discussed in relation to the analysis of correlations (Ref. [26], p. 1641) and thermodynamical properties (Ref. [27], p. 3911) of a confined gas of harmonically interacting spin-polarized fermions.

The many-body variational principle for path integrals was also used recently in order to calculate the ground-state energy and the optical absorption spectrum of a many-polaron system, confined to a quantum dot (Ref. [28], p. 306).

The remainder of this paper addresses the question *which choice of model actions is allowed* in order to treat specific systems of interacting bosons and fermions. I will give some examples, illustrating that the applicability of the many-body variational principle for path integrals crucially depends on whether or not a model system possesses the proper symmetry properties with respect to permutations of identical particles. The requirements analyzed in this article are qualitatively new as compared to the Feynman variational principle of Refs. [1–3].

3 Many-Body Variational Principle for Path Integrals

Let a many-fermion system be described by the action functional $S[\bar{\mathbf{x}}(t)]$, where $\bar{\mathbf{x}} \equiv \{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ are the coordinate vectors of fermions. The partition function Z_F of a many-fermion system can be expressed as a path integral:

$$Z_F = \sum_P \frac{(-1)^P}{N!} \int d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}\,(t) \exp\left\{-S\left[\bar{\mathbf{x}}\,(t)\right]\right\}, \tag{4}$$

where the summation is over all elements P of the permutation group. The weight $(-1)^P$ is the character of the representation, i.e. $+1$ for even permutations and -1 for odd permutations (for the case of fermions).

3.1 Model Systems with Local Potentials

In Ref. [22], a many-body problem was analyzed for a local potential $V(\bar{\mathbf{x}})$ (including interparticle interactions) with the action functional in the imaginary-time representation

$$S\left[\bar{\mathbf{x}}\,(t)\right] = \frac{1}{\hbar} \int_0^{\hbar\beta} dt \left[\frac{m}{2} \sum_{j=1}^{N} \dot{\mathbf{x}}_j^2\,(t) + V\left(\bar{\mathbf{x}}\,(t)\right)\right]. \tag{5}$$

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Note that this action is invariant under the permutations of any two fermions at any (imaginary) time, since the potential cannot make a distinction between identical particles.

If the potential $V(\bar{\mathbf{x}}(t))$ is invariant with respect to the permutations of the *Cartesian components of the particle coordinates* [22,23], the many-body propagator is obtained by four *independent* processes per pair of particles, defined on a state space (D_n^3 in the notations of Ref. [22]) with well-defined boundary conditions (see Eqs. (4.16) and (4.17) in Ref. [22] for details). These processes were shown to give *positive* contributions to the propagator. Hence, the propagator itself is *positive* on D_n^3, implying that the Jensen-Feynman inequality can be used to estimate the partition function for interacting identical particles.[b] The partition function can then be represented (apart from a normalizing factor) in the form

$$Z_F = \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\,(t) \exp\left\{-S\left[\bar{\mathbf{x}}\,(t)\right]\right\}, \;\; \bar{\mathbf{x}}(t) \in D_n^3. \tag{6}$$

Consider now a model system with the action functional in the imaginary-time representation

$$S_M\left[\bar{\mathbf{x}}\,(t)\right] = \frac{1}{\hbar}\int_0^{\hbar\beta} dt \left[\frac{m}{2}\sum_{j=1}^{N} \dot{\mathbf{x}}_j^2\,(t) + V_M\left(\bar{\mathbf{x}}\,(t)\right)\right], \tag{7}$$

where the *model* potential $V_M(\bar{\mathbf{x}})$ contains some variational parameters, and allows for an analytical calculation of the path integral. Suppose furthermore that it is invariant with respect to the permutations of the components of the particle positions. The path-integral expression for the partition function of the model system is thus:

$$Z_M = \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\,(t) \exp\left\{-S_M\left[\bar{\mathbf{x}}\,(t)\right]\right\}, \;\; \bar{\mathbf{x}}(t) \in D_n^3. \tag{8}$$

One can represent (6) as follows:

[b] If the potential is only invariant under permutations of the particle coordinates, the subprocesses are not linearly independent, and transitions between the subprocesses have to be taken into account. The actual analysis in terms of the state space D_n^3 is then only feasible in practice for a very limited number of fermions. In this case, an overcomplete space covered by all even permutations of the particle coordinates is more appropriate.

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$$\begin{aligned} Z_F &\equiv \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\,(t) \exp\left\{-S_M\left[\bar{\mathbf{x}}\,(t)\right] - \left(S\left[\bar{\mathbf{x}}\,(t)\right] - S_M\left[\bar{\mathbf{x}}\,(t)\right]\right)\right\} \\ &= Z_M \langle \exp\left\{-\left(S\left[\bar{\mathbf{x}}\,(t)\right] - S_M\left[\bar{\mathbf{x}}\,(t)\right]\right)\right\}\rangle_{S_M}. \end{aligned} \tag{9}$$

Here, the angular brackets denote the quantum statistical expectation value:

$$\langle \bullet \rangle_{S_M} \equiv \left[Z_M\right]^{-1} \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\,(t) \bullet \exp\left\{-S_M\left[\bar{\mathbf{x}}\,(t)\right]\right\}, \tag{10}$$

analogously to Eq. (2). The key element of this definition is that the path integrals in Eqs. (8-10) are defined on the *same* state space D_n^3, which stems from the symmetry properties of the true action $S\left[\bar{\mathbf{x}}\,(t)\right]$.

Taking into account that the propagators are positive on the domain D_n^3, one obtains the inequality

$$Z_F \geq Z_M \exp\left\{-\langle S\left[\bar{\mathbf{x}}\,(t)\right] - S_M\left[\bar{\mathbf{x}}\,(t)\right]\rangle_{S_M}\right\}, \tag{11}$$

which is readily converted into an upper bound for the free energy

$$F_F \leq F_M + \frac{1}{\beta}\langle S\left[\bar{\mathbf{x}}\,(t)\right] - S_M\left[\bar{\mathbf{x}}\,(t)\right]\rangle_{S_M}. \tag{12}$$

This *many-body variational principle for path integrals* is formally very similar to the Jensen-Feynman inequality (1). The difference between the Eqs. (12) and (1) lies in the definition of the expectation values. In (11) and (12) the expectation value (10) is defined over a subdomain D_n^3 of the configuration space, whereas the expectation value (2) in (1) is defined over the full configuration space. However, because the symmetry properties allow to unfold the state space into the full configuration space, the restriction to the state space can be omitted in the calculation. The state space (D_n^3 in this example) only serves the goal to check whether the action and the trial action have the correct symmetry properties.

3.2 Model Systems with Retarded Effective Interactions

The action functional $S[\bar{\mathbf{x}}(t)]$ of the system under study can contain a retarded effective interaction. This is the case, e.g. for a system of N polarons after the phonon variables have been integrated out. Such many-fermion systems substantially differ from those considered above in subsection 3.1, and a different class of model systems seems to be appropriate. For this purpose,

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we consider a model system consisting of fermions interacting with *auxiliary fictitious particles*.

Such a model system has the action functional in the imaginary-time representation

$$S_M = \frac{1}{\hbar} \int_0^{\hbar\beta} L_M(t)\, dt. \tag{13}$$

The model "Lagrangian" is chosen in the form:

$$L_M = L_F(\bar{\mathbf{x}}) + L_f(\bar{\mathbf{y}}) + L_{F-f}(\bar{\mathbf{x}}, \bar{\mathbf{y}}), \tag{14}$$

where $\{\mathbf{x}_j\} \equiv \bar{\mathbf{x}}$ are the coordinate vectors of the fermions, and $\{\mathbf{y}_j\} \equiv \bar{\mathbf{y}}$ are the coordinate vectors of the fictitious particles. The "Lagrangians" $L_F(\bar{\mathbf{x}})$, $L_f(\bar{\mathbf{y}})$ and $L_{F-f}(\bar{\mathbf{x}}, \bar{\mathbf{y}})$ describe fermions, fictitious particles, and the interaction between the fermions and the fictitious particles, respectively. Here, the discussion is limited to the case of *distinguishable* fictitious particles for the sake of simplicity.

The partition function Z_M of the model system can be written as the following path integral:

$$Z_M = \sum_P \frac{\xi^P}{N!} \int d\bar{\mathbf{x}} \int d\bar{\mathbf{y}} \int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(t) \int_{\bar{\mathbf{y}}}^{\bar{\mathbf{y}}} D\bar{\mathbf{y}}(t) \exp\{-S_M\}. \tag{15}$$

Integrating out the coordinates of the fictitious particles, the partition function (15) takes the form

$$Z_M = Z_0 Z_f, \tag{16}$$

$$Z_0 = \sum_P \frac{\xi^P}{N!} \int d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{P\bar{\mathbf{x}}} D\bar{\mathbf{x}}(t) \exp\{-S_0[\bar{\mathbf{x}}(t)]\}, \tag{17}$$

where Z_f is the partition function of the system of fictitious particles:

$$Z_f = \int d\bar{\mathbf{y}} \int_{\bar{\mathbf{y}}}^{\bar{\mathbf{y}}} D\bar{\mathbf{y}}(t) \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} L_f(\bar{\mathbf{y}})\right\}, \tag{18}$$

and $S_0[\bar{\mathbf{x}}(t)]$ is an effective action which only depends on the fermion variables,

$$S_0[\bar{\mathbf{x}}(t)] \equiv \frac{1}{\hbar} \int_0^{\hbar\beta} (L_F(t)\, dt + \Phi_0[\bar{\mathbf{x}}(t)]). \tag{19}$$

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The last term in (19) is referred to as the *influence phase* of the fictitious particles. It is defined as

$$\exp\left\{-\Phi_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right\} \equiv$$
$$\equiv \left[Z_f\right]^{-1} \int d\bar{\mathbf{y}} \int_{\bar{\mathbf{y}}}^{\bar{\mathbf{y}}} D\bar{\mathbf{y}}\left(t\right) \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} \left[L_f(\bar{\mathbf{y}}) + L_{e-f}(\bar{\mathbf{x}},\bar{\mathbf{y}})\right] dt\right\}. \quad (20)$$

For interaction Lagrangians $L_{e-f}(\bar{\mathbf{x}},\bar{\mathbf{y}})$ which are quadratic in $\bar{\mathbf{y}}$, the influence phase can be shown to take the form of a *retarded effective interaction*:

$$\Phi_0\left[\bar{\mathbf{x}}(t)\right] = \int\limits_0^{\hbar\beta} dt \int\limits_0^{\hbar\beta} ds K(t,s) \mathbf{X}\left(t\right) \cdot \mathbf{X}\left(s\right), \quad (21)$$

where $K(t,s)$ depends on two time variables (t,s), while $\mathbf{X}\left(t\right)$ is a linear function of the fermion coordinates $\bar{\mathbf{x}}\left(t\right)$ (see the next section for specific examples).

If the action functional $S\left[\bar{\mathbf{x}}\left(t\right)\right]$ of the system under study satisfies the permutation symmetry conditions discussed in the previous subsection, its partition function can be represented as a path integral over the space state D_n^3 in the form (6):

$$\begin{aligned} Z_F &\equiv \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\left(t\right) \exp\left\{-S_0\left[\bar{\mathbf{x}}\left(t\right)\right] - \left(S\left[\bar{\mathbf{x}}\left(t\right)\right] - S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right)\right\}, \\ &= Z_0 \langle \exp\left\{-\left(S\left[\bar{\mathbf{x}}\left(t\right)\right] - S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right)\right\}\rangle_{S_0}. \end{aligned} \quad (22)$$

If the model action $S_0\left[\bar{\mathbf{x}}\left(t\right)\right]$ also possesses the above symmetry properties with respect to permutations, its partition function (17) can also be written in the form of a path integral over the domain D_n^3,

$$Z_0 = \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\left(t\right) \exp\left\{-S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right\}, \quad (23)$$

and the quantum statistical expectation value in (22) can be defined as

$$\langle\bullet\rangle_{S_0} \equiv \left[Z_0\right]^{-1} \int_{D_n^3} d\bar{\mathbf{x}} \int_{\bar{\mathbf{x}}}^{\bar{\mathbf{x}}} D\bar{\mathbf{x}}\left(t\right) \bullet \exp\left\{-S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right\}, \quad (24)$$

analogously to the definition (2). The fact that the propagators are positive in the integration domain D_n^3 guarantees that the inequality

$$Z_F \geq Z_0 \exp\left\{\langle-\left(S\left[\bar{\mathbf{x}}\left(t\right)\right] - S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\right)\rangle_{S_0}\right\} \quad (25)$$

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holds true. Consequently we obtain an upper bound for the free energy similar to Eq. (12):

$$F_F \leq F_v \equiv F_0 + \frac{1}{\beta} \langle S\left[\bar{\mathbf{x}}\left(t\right)\right] - S_0\left[\bar{\mathbf{x}}\left(t\right)\right]\rangle_{S_0}, \tag{26}$$

where $F_0 = -(\ln Z_0)/\beta$ and $F_F = -(\ln Z_F)/\beta$.

Because of the presence of the retarded action (21) resulting from the elimination of the fictitious particles, one should guarantee that the functional $S_0\left[\bar{\mathbf{x}}\left(t\right)\right]$ has the required symmetry with respect to permutations which allows that the many-body processes, related to the quantum statistical expectation value (24), are restricted to the state space D_n^3 at any time. This condition is an essential ingredient for the justification of the *many-body variational principle for path integrals* (12). Like in the case (12) of local potentials, the upper bound (26) to the free energy is formally very similar to the Jensen-Feynman inequality (1): the difference lies again in the definition of the expectation values. In (25) and (26) the expectation value (24) is defined over the subdomain D_n^3 of the configuration space, whereas the expectation value (2) in (1) is defined over the full configuration space. However, like in the previous subsection, the state space (D_n^3 in this case) is only needed to check whether the symmetry of the action and the trial action allows to apply the inequality. The calculation can be performed over the total configuration space by unfolding the state space.

4 Examples: Non-Interacting Fermions as a Test Case for a Many-Body Variational Principle with Path Integrals

4.1 Model Syste with Each Fermion Harmonically Interacting with One Fictitious Particle

In order to illustrate the applicability of the many-body variational principle for path integrals (26), and in particular the need of the correct symmetry requirements for the model action, we first consider a very simple system of $N = \sum_{\sigma=\pm 1/2} N_\sigma$ non-interacting fermions, described by the Lagrangian

$$L_F = \frac{m}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \dot{\mathbf{x}}_{j,\sigma}^2, \tag{27}$$

where N_σ is the number of electrons with spin component $\sigma = \pm 1/2$. The ground-state energy for the system with the classical "Lagrangian" (27) is

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elementary:

$$E = \frac{3}{5} E_F, \quad E_F \equiv \frac{\hbar^2 k_F^2}{2m}, \tag{28}$$

with the Fermi wave number k_F and the Fermi energy E_F.

We now examine whether the many-body variational principle for path integrals (26) indeed provides an upper bound to the correct ground-state energy (28).

For the model system (14) we choose a Lagrangian L_M, in which each fermion harmonically interacts with *one fictitious particle*. We do this uncritically, deliberately overlooking the problem of the required symmetry of the state space of the model action and choose

$$\begin{aligned} L_M =& \frac{m}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \dot{\mathbf{x}}_{j,\sigma}^2 \\ &+ \frac{M}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \dot{\mathbf{y}}_{j,\sigma}^2 + \frac{k}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \left(\mathbf{x}_{j,\sigma} - \mathbf{y}_{j,\sigma}\right)^2, \end{aligned} \tag{29}$$

where M is the mass of the fictitious particles, and k is the force constant of the elastic bond between a fermion and its accompanying fictitious particle. We introduce the following notations:

$$w = \sqrt{\frac{k}{M}}, \quad v = \sqrt{\frac{k}{\mu}}, \quad \mu = \frac{mM}{m+M}.$$

For this particular case, the elimination of the fictitious particles leads to the influence phase (20):

$$\begin{aligned} \Phi_0 \left[\bar{\mathbf{x}}(t)\right] =& -\frac{Mw^3}{8\hbar} \int_0^{\hbar\beta} dt \int_0^{\hbar\beta} ds \frac{\cosh w \left(|t-s| - \frac{\hbar\beta}{2}\right)}{\sinh \frac{1}{2}\hbar\beta w} \\ &\times \sum_{\sigma=\pm 1} \sum_{j=1}^{N_\sigma} [\mathbf{x}_{j,\sigma}(t) - \mathbf{x}_{j,\sigma}(s)]^2, \end{aligned} \tag{30}$$

with a quadratic effective retarded self-interaction for each fermion.

Then we apply the many-body variational principle for path integrals (26) naively to the chosen model system. The free energy F_v from this inequality is calculated analytically. The parameters M and k of the model "Lagrangian" (14) are then found by minimizing the value of the supposed upper bound

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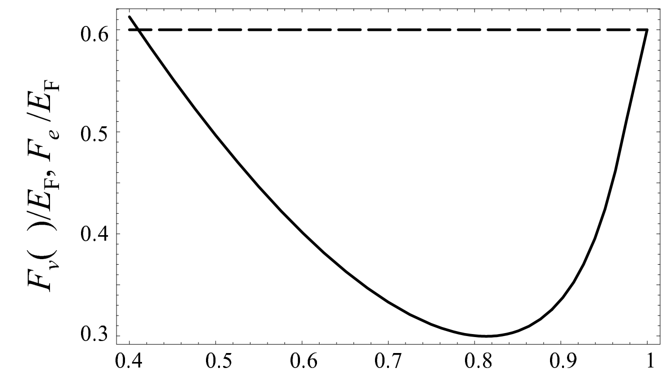

Figure 1. Free energy $F_v(\theta)$ ($\theta = w/v$) for non-interacting fermions [according to the inequality (26)] (solid line) compared with the exact free energy F_e (dashed line) at the optimal value of the variational frequency parameter $v = 1.83$ (in units of $E_F/\hbar$, where $E_F = 49$ meV is the Fermi energy for the density $n_e = 5 \times 10^{19}$ cm^{-3}, rather arbitrarily chosen); $\beta = 16.4$ (in units of E_F^{-1}). The mass m of a fermion is taken to be m_0, the bare electron mass.

F_v. This calculation has shown that the many-body variational principle for path integrals (26) is *violated* for this model system, as clearly illustrated in Fig. 1.

What was wrong in the above approach? The answer is immediate: "Of course, we forgot to check whether the model action has the required symmetry!" The model "Lagrangian" (29) is *not symmetrical* with respect to the permutations of the fermion coordinates $\mathbf{x}_{j,\sigma}$, because each of them is linked with a particular fictitious particle.

4.2 Model System with Each Fermion Having Equal Elastic Bonds with All Fictitious Particles

As a second example, we study the many-body variational principle for path integrals (26) for $N = \sum_{\sigma=\pm 1/2} N_\sigma$ non-interacting electrons in a parabolic confinement described by the Lagrangian (in the imaginary-time variable)

$$L = \frac{m}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \left(\dot{\mathbf{x}}_{j,\sigma}^2 + \Omega_0^2 \mathbf{x}_{j,\sigma}^2 \right) . \tag{31}$$

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In particular, the case $\Omega_0 \to 0$ will be analyzed (a translationally invariant system, equivalent to the free-fermion model in subsection 4.1). The exact ground-state energy of this system can immediately be written down:

$$E_0\left(\Omega_0, N\right) = \hbar\Omega_0 \sum_{\sigma=\pm 1/2} \left\{ N_\sigma \left[n_0\left(N_\sigma\right) + \frac{5}{2} \right] \right.$$
$$\left. - \frac{1}{4} N_0\left(n_0\left(N_\sigma\right)\right)\left[n_0\left(N_\sigma\right) + 4\right] \right\}. \tag{32}$$

Here, $n_0(N_\sigma)$ is the number of the upper fully occupied energy level for N_σ fermions with spin component σ. The number of fermions in all closed shells $[N_0(n_0(N_\sigma)) \leq N_\sigma]$ is

$$N_0\left(n_0\right) \equiv \sum_{n=0}^{n_0} \frac{(n+1)(n+2)}{2} = \frac{1}{6}\left(n_0+1\right)\left(n_0+2\right)\left(n_0+3\right). \tag{33}$$

A model system is now considered, which consists of particles in a harmonic confinement potential with elastic interparticle interactions as studied in Ref. [29]. The "Lagrangian" of this model system is chosen in the form

$$\begin{aligned} L_M =& \frac{m}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \left(\dot{\mathbf{x}}_{j,\sigma}^2 + \Omega^2 \mathbf{x}_{j,\sigma}^2\right) + \frac{m\omega^2}{4} \sum_{\sigma,\tau=\pm 1/2} \sum_{j,l=1}^{N_\sigma} \left(\mathbf{x}_{j,\sigma} - \mathbf{x}_{l,\tau}\right)^2 \\ &+ \frac{M}{2} \sum_{l=1}^{N_B} \left(\dot{\mathbf{y}}_j^2 + \Omega_B^2 \mathbf{y}_j^2\right) + \frac{M\omega_B^2}{4} \sum_{j=1}^{N_B} \sum_{l=1}^{N_B} \left(\mathbf{y}_j - \mathbf{y}_l\right)^2 \\ &+ \frac{k}{2} \sum_{\sigma=\pm 1/2} \sum_{j=1}^{N_\sigma} \sum_{l=1}^{N_B} \left(\mathbf{x}_{j,\sigma} - \mathbf{y}_l\right)^2 . \end{aligned} \tag{34}$$

The frequencies Ω, ω, Ω_B, ω_B, the mass M of fictitious particles, and the force constant k are treated as *variational parameters*. It is important to stress, that in this model system each fermion has identical elastic bonds with *all* fictitious particles, and therefore permutations of the fermion coordinates leave the "Lagrangian" (34) invariant.

After integration over the paths of the fictitious particles, the partition function (16) becomes

$$Z_f = \left[\sinh\left(\frac{\hbar\beta\tilde{\Omega}_B}{2}\right)\right]^3 \left[\sinh\left(\frac{\hbar\beta w_B}{2}\right)\right]^{3N_B-3}, \tag{35}$$

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with

$$\tilde{\Omega}_B = \sqrt{\Omega^2 + \frac{kN_B}{m}}, \quad w_B = \sqrt{\Omega^2 - N_B\omega^2 + \frac{kN_B}{m}}. \tag{36}$$

The action (19) in the imaginary time representation takes the form

$$S_0\left[\bar{\mathbf{x}}(t)\right] \equiv S_{F0}\left[\bar{\mathbf{x}}(t)\right] + \Phi_0\left[\bar{\mathbf{x}}(t)\right], \tag{37}$$

$$S_{F0}\left[\bar{\mathbf{x}}(t)\right] = \frac{1}{\hbar}\int_0^{\hbar\beta} dt \left[\sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\frac{m}{2}\dot{\mathbf{x}}_{j,\sigma}^2(t) + \frac{m\omega^2 N^2}{2}\mathbf{X}^2\right], \tag{38}$$

with the coordinate

$$\mathbf{X} \equiv \sum_{\sigma=\pm 1/2}\sum_{j=1}^{N_\sigma}\mathbf{x}_{j,\sigma}, \tag{39}$$

and the "influence phase" (20) for the present model becomes

$$\Phi_0\left[\bar{\mathbf{x}}(t)\right] = \frac{k^2N^2N_B^2}{4m_B\hbar\tilde{\Omega}_B}\int_0^{\hbar\beta} dt \int_0^{\hbar\beta} ds \frac{\cosh\left[\tilde{\Omega}_B\left(|t-s| - \frac{\hbar\beta}{2}\right)\right]}{\sinh\left(\frac{\hbar\beta\tilde{\Omega}_B}{2}\right)}\mathbf{X}(t)\cdot\mathbf{X}(s). \tag{40}$$

As distinct from (29), this model Lagrangian (34) is *invariant with respect to permutations of the components of all fermion coordinates.* Hence, for the chosen model system the symmetry conditions on the action are fulfilled (as formulated in subsection 4.1), which ensures the validity of the many-body variational principle for path integrals (26).

The functional [resulting from (26) at zero temperature] for the ground-state energy of N fermions in a parabolic confinement with the confinement frequency Ω_0 takes the form

$$\begin{aligned} E_v\left(\Omega_1, \Omega_2, w, w_B\right) = \hbar\Bigg\{ & \frac{\Omega_0^2 + w^2}{2w^2}\left[\tilde{E}(w, N) - \frac{3}{2}w\right] + \frac{3}{2}\left(\Omega_1 + \Omega_2 - w_B\right) \\ & + \frac{3}{4}\left(\Omega_0^2 - \Omega_1^2 - \Omega_2^2 + w_B^2\right)\sum_{i=1}^{2}\frac{a_i^2}{\Omega_i} + \frac{3\gamma^2}{4w_B}\sum_{i=1}^{2}\frac{a_i^2}{\Omega_i\left(\Omega_i + w_B\right)}\Bigg\}, \end{aligned} \tag{41}$$

where the following notations are used:

$$a_1 = \left(\frac{\Omega_1^2 - w_B^2}{\Omega_1^2 - \Omega_2^2}\right)^{1/2}, \quad a_2 = \left(\frac{w_B^2 - \Omega_2^2}{\Omega_1^2 - \Omega_2^2}\right)^{1/2}, \tag{42}$$

$$\gamma = \left[\left(\Omega_1^2 - w_B^2\right)\left(w_B^2 - \Omega_2^2\right)\right]^{1/2}, \tag{43}$$

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and

$$\tilde{E}(w,N)=\hbar w\sum_{\sigma=\pm1/2}\left\{N_\sigma\left[n_0(N_\sigma)+\frac{5}{2}\right]\right.$$
$$\left.-\frac{1}{4}N_0(n_0(N_\sigma))\left[n_0(N_\sigma)+4\right]\right\}. \tag{44}$$

The difference between the upper bound to the ground-state energy (41) and the exact ground-state energy (32) is clearly positive:

$$E_v(\Omega_1,\Omega_2,w,w_B)-E_0(\Omega_0,N)=\frac{3\hbar}{4}\frac{(\Omega_0-z)^2}{z}, \tag{45}$$

with

$$z=\frac{\Omega_1\Omega_2+\Omega_0^2}{\Omega_1+\Omega_2}, \tag{46}$$

and it follows from (45) that the inequality

$$E_v(\Omega_1,\Omega_2,w,w_B)\geq E_0(\Omega_0,N) \tag{47}$$

holds true for any values of the variational parameters, *in accordance with the many-body variational principle for path integrals* (26).

The minimal value of the functional (41), which is achieved at $z=\Omega_0$, coincides with the exact ground-state energy (32) of N non-interacting fermions in a parabolic confinement with the frequency Ω_0. This result confirms the applicability of the many-body variational principle for path integrals (26) to the many-fermion system under consideration, with a model system, whose "Lagrangian" (34) is symmetric under the permutations of the components of the fermion positions.

Thus, the many-body variational principle for path integrals (26) is satisfied for a system of non-interacting fermions in a parabolic confinement potential (including the translationally invariant case $\Omega_0=0$), when the model system with the "Lagrangian" (34) is considered.

Clearly, the Lagrangian (31) was not considered for its own sake, since it is trivial to treat. It was merely presented as a test case to illustrate our many-body variational principle for path integrals with two non-trivial trial actions which elucidate the crucial role of the correct symmetry requirements.

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5 Conclusions

Summarizing, the applicability of the many-body variational principle for path integrals (26) crucially depends on the symmetry of the model system with respect to permutations of identical particles.

The invariance of the action functional $S_0[\bar{\mathbf{x}}(t)]$ and of the model action with respect to permutations of components of the positions of any two fermions at any (imaginary) time ensures that the fermion propagator is positive on the state space D_n^3.

It should be noted that these rather stringent symmetry conditions are used as an example. A more general variational principle for identical particles, not limited to D_n^3 but to a much larger subspace of the configuration space, will be presented in future publications.

The main result of the present analysis is that a many-body variational principle for path integrals (26) can be found in the framework of the many-body path-integral approach, even for retarded effective interactions, provided that the model action and the true action have the appropriate symmetry properties under permutations of the particle coordinates.

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