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Systematic Improvement of Hartree–Fock–Bogoliubov Approximation with Exponentially Fast Convergence from Variational Perturbation Theory

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The recently developed exponentially fast convergent variational perturbation theory of the anharmonic oscillator is generalized to a systematic extension of the Hartree–Fock–Bogoliubov approximation of many-particle systems with a similar convergence. The relation with the effective action approach based on bilocal Legendre transforms is exhibited.

I. INTRODUCTION

Variational perturbation theory [1] is a systematic extension of a variational method developed some years ago by Feynman and Kleinert [2], and others [3], and converts divergent perturbation expansions for energy levels and free energies of a quantum mechanical anharmonic oscillator into exponentially fast converging expansions for all coupling strength [1, 4]. This is achieved by perturbing around an oscillator with a trial frequency Ω^2, which is optimized at each order N of the expansion. The optimal value Ω_N is defined by the requirement that it minimizes the dependence of the energy on Ω. Up to the high order $N=15$, the odd approximants are optimal at a unique minimum of the energy as a function of Ω. For even orders there exists no minimum, but the Ω^2-dependence can nevertheless be minimized at a unique saddle point. A somewhat worse approximation is obtained by evaluating even approximations at the minimum of the previous odd approximation.

In this note we reformulate and generalize the procedure in such a way that it becomes applicable to field theories of many-body systems. We derive a set of equations which systematically improve the standard Hartree–Fock–Bogoliubov approximation to many-body systems.

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II. REFORMULATION AND GENERALIZATION OF VARIATIONAL PERTURBATION THEORY

For the anharmonic oscillator with a euclidean action

$$\mathcal{A} = \mathcal{A}_\omega + \mathcal{A}^{\text{int}} \equiv \frac{1}{2}\int d\tau\,[\dot{x}^2(\tau) + \omega^2 x^2(\tau)] + \int d\tau \left[\frac{g_3}{3!}\,x^3(\tau) + \frac{g_4}{4!}\,x^4(\tau)\right], \quad (1)$$

variational perturbation theory may be summarized as follows: The free energy of a quantum mechanical system is written as

$$F = F^0 + F^{\text{int}}, \quad (2)$$

where F^0 is the free energy of the harmonic oscillator

$$F^0 = -\frac{1}{2\beta}\,\text{Tr}\log(G_0). \quad (3)$$

The parameter β is the inverse temperature $\beta = 1/k_B T$, with $k_B =$ Boltzmann constant, and $G_0(\tau, \tau')$ denotes the imaginary-time correlation function

$$G_0(\tau, \tau') = (-\partial_\tau^2 + \omega^2)^{-1}\,(\tau, \tau') \quad (4)$$

of the harmonic oscillator, its explicit finite-temperature form being, in natural units with $h = 1$,

$$G_0(\tau, \tau') = G_\omega(\tau - \tau') = \frac{1}{2\omega}\,\frac{\cosh\omega(|\tau - \tau'| - \beta/2)}{\sinh(\omega\beta/2)}, \quad (5)$$

which has the limit $e^{-\omega|\tau-\tau'|}/2\omega$ for $T \to 0$. The associated free energy is found from the formula

$$F^0 = -\frac{1}{2\beta}\int_0^\infty \frac{d\tau}{\tau}\,\text{Tr}[e^{-\tau G_0^{-1}}]. \quad (6)$$

The right-hand side is regular at $\tau = 0$ if the trace is evaluated in dimensional regularization, yielding for the harmonic oscillator

$$F^0 = \frac{1}{\beta}\log[2\sinh(\beta\omega/2)], \quad (7)$$

which tends to the ground-state energy $\omega/2$ for $T \to 0$.

The second term in (2) is the free energy caused by the interactions. It possesses a divergent expansion in powers of the interaction strength calculated by the rules

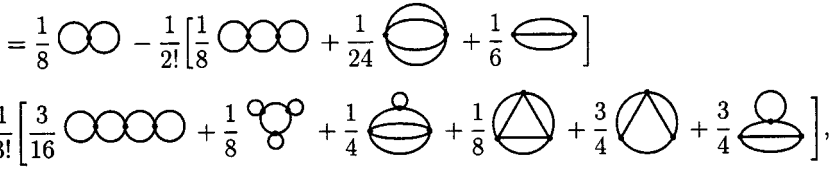
of perturbation theory. Introducing the notation $\langle \cdots \rangle_\omega$ for the thermal expectation values within the harmonic oscillator of frequency ω, expansion reads

$$\beta F^{\text{int}} = \langle \mathscr{A}^{\text{int}} \rangle_\omega - \frac{1}{2!} \langle (\mathscr{A}^{\text{int}})^2 \rangle_{\omega,c} + \frac{1}{3!} \langle (\mathscr{A}^{\text{int}})^3 \rangle_{\omega,c} - \cdots . \tag{8}$$

The subscript c indicates that the cumulants of the expectation values have to be taken, i.e.

$$\begin{aligned} \langle (\mathscr{A}^{\text{int}})^2 \rangle_{\omega,c} &= \langle (\mathscr{A}^{\text{int}})^2 \rangle_\omega - \langle \mathscr{A}^{\text{int}} \rangle_\omega^2 , \\ \langle (\mathscr{A}^{\text{int}})^3 \rangle_{\omega,c} &= \langle (\mathscr{A}^{\text{int}})^3 \rangle_\omega - 3 \langle (\mathscr{A}^{\text{int}})^2 \rangle_\omega \langle \mathscr{A}^{\text{int}} \rangle_\omega + 2 \langle \mathscr{A}^{\text{int}} \rangle_\omega^3 , \\ &\vdots \end{aligned} \tag{9}$$

For the x^3- and x^4-interaction at hand, the perturbation expansion (8) may be displayed most easily in terms of connected Feynman diagrams. Using Wick's rule we find, up to the order $N = 3$,

$\beta F_3^{\text{int}} =$ 

(10)

where vertices represent coupling constants $g_3/3!$, $g_4/4!$, depending on the number of lines emerging. The lines stand for the harmonic-oscillator correlation function G_0.

The interactions change $G_0(\tau, \tau')$ to $G(\tau, \tau')$, which may also be expanded into a power series in the coupling strengths $g_3/3!$, $g_4/4!$. The diagrams contributing to $G(\tau, \tau')$ are efficiently obtained from the interaction diagrams in (10) in two steps: First one differentiates the interaction diagrams with respect to G_0, which is most easily be done graphically by removing a single line in all possible ways. From the resulting diagrams one further removes all those which are one-particle-reducible, i.e., which fall apart when cutting a single line. The remaining one-particle-irreducible diagrams yield the self-energy $\Sigma(\tau, \tau')$. In a second step one forms

$$G(\tau, \tau') = [\, (-\partial_\tau^2 + \omega^2)\, \delta(\tau - \tau') + \Sigma(\tau, \tau') \,]^{-1} (\tau, \tau'), \tag{11}$$

or simpler

$$G^{-1}(\tau, \tau') \equiv G_0^{-1}(\tau, \tau') + \Sigma(\tau, \tau'). \tag{12}$$

This corresponds to summing up all self-energy diagrams in a geometric series

$$G \to G_0 - G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 - G_0 \Sigma G_0 \Sigma G_0 \Sigma G_0 + \cdots . \tag{13}$$

For the development to come it will be useful to consider $F = F^0 + F^{\text{int}}$ as a functional of the harmonic-oscillator correlation function $G_0(\tau, \tau')$, to be indicated by a functional argument G_0.

A variational perturbation expansion is obtained from the expansion (10) by the following steps:

1. We use (12) to rewrite $F[G_0]$ in (3) trivially as $F[(G^{-1} - \Sigma)^{-1}]$. This is expanded into a power series in Σ up to the same order N to which the perturbation series for F^{int} is known. With the interaction (10), we go to Σ^3.

2. The truncated expression

$$F_N[G, \Sigma] = \sum_{n=0}^{N} \frac{1}{n!} F^{(n)}[G] \Sigma^n \tag{14}$$

is extremized in G, varying $\Sigma = \Sigma[G]$ as a functional of G in accordance with (12) which implies:

$$\frac{\delta \Sigma}{\delta G} = -G^{-2}. \tag{15}$$

Variational perturbation theory is based on the observation that the complete expansion of $F[(G^{-1} - \Sigma)^{-1}] \equiv F[G^0]$ is certainly independent of G. The truncated expansion $F_N[G, \Sigma[G]]$, on the other hand, *does* depend on G. At any given order N, the final result is approached best by choosing a correlation function $G = G_N$ for which $F_N[G, \Sigma[G]]$ has the smallest G-dependence.

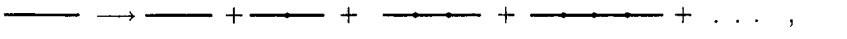
For the free energy (3) of the anharmonic oscillator, the expansion of $F^0[(G^{-1} - \Sigma)^{-1}]$ yields, up to $N = 3$,

$$\beta F^0[G, \Sigma] = \tfrac{1}{2} \operatorname{Tr} \log G^{-1} - \tfrac{1}{2} \operatorname{Tr}(G\Sigma) - \tfrac{1}{4} \operatorname{Tr}(G\Sigma)^2 - \tfrac{1}{6} \operatorname{Tr}(G\Sigma)^3 - \cdots. \tag{16}$$

The same reexpansion is performed for the interaction energy (10), most easily graphically. The replacement $G_0 \to (G^{-1} - \Sigma)^{-1}$ replaces each propagator into a geometric series

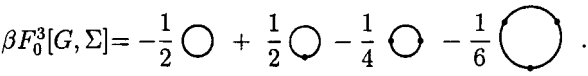
$$G_0 \to G + G\Sigma G + G\Sigma G\Sigma G + G\Sigma G\Sigma G\Sigma G + \cdots, \tag{17}$$

which in the Feynman diagram corresponds to an exchange



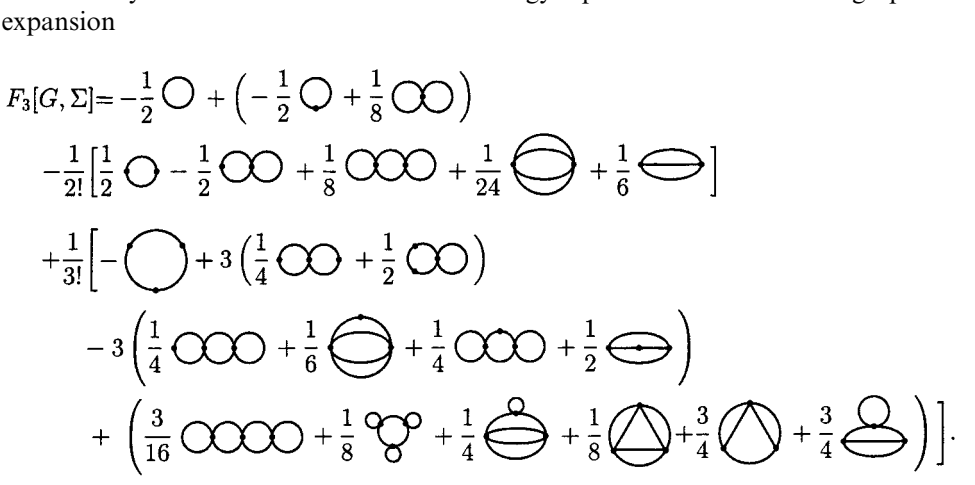
(18)

where the lines on the right-hand side stand for the full propagator, and a point indicates the insertion of a self energy Σ. If we denote Tr log G by a single loop, the expansion (16) can be represented graphically by



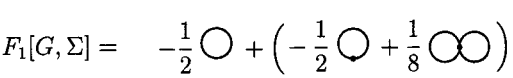
(19)

In this way we find for the total free energy up to order $N=3$ the graphical expansion



(20)

Let us first optimize the expansion for $N=1$. The free energy $F_1[G,\Sigma]$ reads graphically



(21)

and analytically,

$$\beta F_1[G,\Sigma] = -\frac{1}{2}\,\mathrm{Tr}\log G - \frac{1}{2}\,\mathrm{Tr}(\Sigma G) + 3\,\frac{g_4}{4!}\int_0^\beta d\tau\, G^2(\tau,\tau). \tag{22}$$

Extremizing this in G with the help of (15), we obtain the equation for the self-energy

$$\Sigma(\tau,\tau) = \delta(\tau-\tau')4\cdot 3\,\frac{g_4}{4!}\,G(\tau,\tau). \tag{23}$$

The self-energy is obtained from the interaction term in $F_1[G,\Sigma]$ by a differentiation with respect to $G[\tau,\tau']$, which in the graphical representation (21) removes from the interaction graph a single leg in all possible ways,

(24)

This equation is solved recursively together with (12). We recognize the recursive procedure typical for the self-consistent Hartree–Fock–Bogoliubov approximation. The factor 3 in (22) and (23) accounts for the three characteristic contributions to

the approximaμtion found by those three authors. The three contributions correspond to the three Wick contractions in the expectation value

$$\langle \mathscr{A}^{\text{int}} \rangle_\omega = \frac{g_4}{4!} \int_0^\beta d\tau \langle x^4(\tau) \rangle_\omega = 3 \times \frac{g_4}{4!} \int_0^\beta d\tau \langle x^2 \rangle_\omega^2 . \tag{25}$$

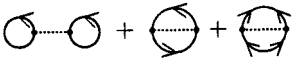
In the anharmonic oscillator, the temporal locality of the interaction $\int_0^\beta d\tau\, x^4(\tau)$ does not permit us to distinguish the three contractions. The difference becomes visible only when considering a more general action in which a two-dimensional harmonic oscillator has a bilocal interaction. Written in terms of complex coordinates $x(\tau) = x_1(\tau) + ix_2(\tau)$, this reads

$$\mathscr{A}^{\text{int}} = \tfrac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau'\, x^*(\tau)\, x^*(\tau')\, V(\tau - \tau')\, x(\tau')\, x(\tau). \tag{26}$$

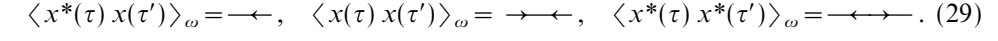
Instead of the expectation value (25), we now find three different contractions

$$\begin{aligned} \langle \mathscr{A}^{\text{int}} \rangle_\omega = \tfrac{1}{2} \int_0^\beta d\tau\, d\tau' \, [& \langle x^*(\tau)\, x(\tau) \rangle_\omega \, V(\tau - \tau') \langle x^*(\tau')\, x(\tau') \rangle_\omega \\ & + \langle x^*(\tau)\, x(\tau') \rangle_\omega \, V(\tau - \tau') \langle x^*(\tau)\, x(\tau') \rangle_\omega \\ & + \langle x^*(\tau)\, x^*(\tau') \rangle_\omega \, V(\tau - \tau') \langle x(\tau)\, x(\tau') \rangle_\omega]. \end{aligned} \tag{27}$$

The first term was introduced by Hartree, the second corresponds to the exchange interaction considered by Fock, and the third is responsible for pairing effects explored first by Bogoliubov. Graphically, these interaction terms are represented by

 . (28)

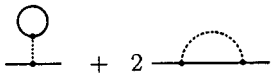
The lines carry an arrow pointing towards the complex-conjugate variable $x^*(\tau)$:

 (29)

For the interaction (26), the lowest-order self-energy is bilocal. To show this explicitly, let $x(\tau)$ be a real variable, the arrows disappear and the last two terms in (27) coincide. A graphical differentiation of the vacuum diagrams (28) yields a self-energy

$$\Sigma(\tau, \tau') = \delta(\tau - \tau') \int_0^\beta d\tau'\, V(\tau - \tau')\, G(\tau', \tau') + 2V(\tau - \tau')\, G(\tau, \tau'). \tag{30}$$

This can be displayed graphically as

$\Sigma(\tau, \tau') =$  (31)

For such a bilocal equation, a recursive solution proceeds by assuming some simple initial $\Sigma(\tau, \tau')$ and solving the eigenvalues equation

$$(-\partial_\tau^2 + \omega^2 - \Sigma)\,\phi_k(\tau) = (-\partial_\tau^2 + \omega^2)\phi_k - \int_0^\beta d\tau'\,\Sigma(\tau, \tau')\,\phi_k(\tau') = \lambda_k \phi_k(\tau). \quad (32)$$

From the solutions, a Green function $G(\tau, \tau')$ is obtained via the spectral representation

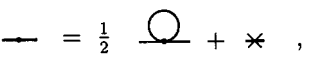
$$G(\tau, \tau') = \sum_k \frac{1}{\lambda_k}\,\phi_k(\tau)\,\phi_k(\tau'). \quad (33)$$

This is reinserted into Eq. (30) to find a new self-energy $\Sigma(\tau, \tau')$, and so on.

The variational procedure can now easily be carried to order $N = 3$. For this we first simplify the graphical expansion (20) by separating the self-energy into the just-derived first-order expression Σ_1 and a remainder

$$\Sigma = \Sigma_1 + \Sigma_R\,. \quad (34)$$

Graphically, this amounts to the replacement

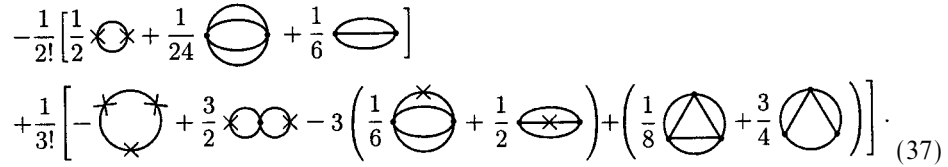
 (35)

The cross symbolizes Σ_R. Then we obtain

$$\beta F_3[G, \Sigma] = \beta F_1[G, \Sigma] + \beta\,\Delta F_3[G, \Sigma_R], \quad (36)$$

with the much simpler set of graphs

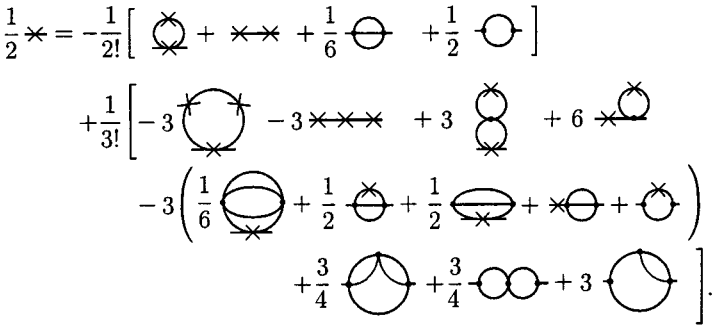
$\Delta F_3[G, \Sigma] =$

 (37)

Extremizing $F_3[\Sigma, G]$ with respect to G, we find

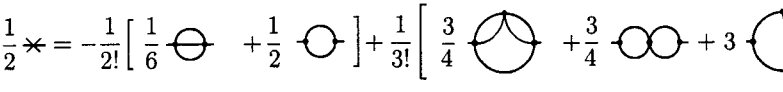
$$\frac{\delta}{\delta G}\,\beta F_3[G, \Sigma[G]] = \frac{1}{2}\,\Sigma_R. \tag{38}$$

The diagrams in $\beta\,\Delta F_3[G, \Sigma_R]$ are differentiated again by removing successively a line from each graph. In addition, the functional derivatives of Σ_R creates a four-point function which we denote by a crossed vertex with four legs. As a result, we obtain for Σ_R the diagrammatic expansion:



(39)

The solution proceeds iteratively: We first ignore all diagrams with crosses on the right-hand side and find the lowest approximation to Σ_R:



(40)

This is functionally differentiated with respect to G to obtain the crossed vertex  . The two equations are is reinserted into (39), and so on.

Note that the diagrams of the lowest-order approximation (40) to Σ_R in this iteration scheme are obtained from the diagrams (10) in the initial free energy by removing a single line from all *two-particle-irreducible* diagrams, which are those not falling apart when cutting two lines. Such a self-energy was found in an earlier attempt to systematically extend the Hartree–Fock–Bogoliubov approximation [5], which is superceded by the present scheme, as will be discussed in Section IV.

III. MANY-BODY SYSTEMS

The above theory can easily be generalized to become applicable to field theories of many-body systems. There the typical action reads

$$\mathscr{A} = \int_0^\beta d\tau \left\{ \int d^3x [\psi^*(\mathbf{x}, \tau) \left[-\partial_\tau - \frac{\hat{\mathbf{p}}^2}{2} - V_1(\mathbf{x}) \right] \psi(\mathbf{x}, \tau) \right.$$

$$\left. - \frac{1}{2} \int d^3x\, d^3x'\, \psi^*(\mathbf{x}', \tau)\, \psi(\mathbf{x}', \tau)\, V_2(\mathbf{x}' - \mathbf{x})\, \psi^*(\mathbf{x}, \tau)\, \psi(\mathbf{x}, \tau) \right\}. \quad (41)$$

where $V_1(\mathbf{x})$ and $V_2(\mathbf{x}' - \mathbf{x})$ are time-independent one- and two-body potentials and $\hat{\mathbf{p}}$ is Schrödinger's momentum operator $-i\partial/\partial\mathbf{x}$. The free part of the free energy is now

$$F^0[G_0] = \pm \frac{1}{\beta} \operatorname{Tr} \log G_0^{-1} \quad (42)$$

with the Green function

$$G_0 = \left[\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2} + V_\tau(\mathbf{x}) \right]^{-1}, \quad (43)$$

where the upper and lower signs in (42) hold for bosons and fermions, respectively.

For simplicity, we consider only a fermion system without pairing correlations of the Bogoliubov type, at zero temperature. Let $\phi_k(\mathbf{x})$ denote the eigenfunctions of the time-independent Schrödinger equation

$$\left[\frac{\hat{\mathbf{p}}^2}{2} + V_1(\mathbf{x}) \right] \phi_k(\mathbf{x}) = \lambda_k^0 \phi(\mathbf{x}). \quad (44)$$

At zero temperature, all energy levels below a certain Fermi energy ε_F are filled, all others are empty. Then the zeroth-order Green function has the decomposition

$$G_0(\mathbf{x}, \tau; \mathbf{x}', \tau') = \langle \hat{T}_\tau \hat{\psi}(\mathbf{x}, \tau)\, \hat{\psi}^\dagger(x', \tau') \rangle$$

$$= \Theta(\tau - \tau')\, G_0^{(+)}(\mathbf{x}, \tau; \mathbf{x}', \tau') \pm \Theta(\tau' - \tau)\, G_0^{(-)}(\mathbf{x}, \tau; \mathbf{x}', \tau'), \quad (45)$$

where $\hat{T}_\tau$ is the time-ordering operator, and

$$G_0^{(+)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \langle \hat{\psi}(\mathbf{x}, \tau)\, \hat{\psi}^\dagger(x', \tau') \rangle = \sum_{\lambda_k > \varepsilon_F} e^{-\lambda_k^0(\tau - \tau')} \phi_k(\mathbf{x})\, \phi_k^*(\mathbf{x}'),$$

$$G_0^{(-)}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \langle \hat{\psi}^\dagger(x', \tau')\, \hat{\psi}(\mathbf{x}, \tau) \rangle = \sum_{\lambda_k < \varepsilon_F} e^{\lambda_k^0(\tau - \tau')} \phi_k(\mathbf{x})\, \phi_k^*(\mathbf{x}'). \quad (46)$$

Since the argument of the trace of the logarithm in (42) contains only a single time derivative and is otherwise τ-independent, it can be simplified. In the operator form of the interaction (41), all field operators $\hat{\psi}^\dagger(\mathbf{x}, \tau)$ are normally ordered to the left of all $\hat{\psi}(\mathbf{x}, \tau)$. The equal-time limit of Green functions in the associated Wick

contractions has the time τ slightly before τ', i.e. $\tau = \tau' - \varepsilon$. Then only the occupied states contribute to $G_0(\mathbf{x}\tau; \mathbf{x}', \tau)$:

$$G_0(\mathbf{x}, \tau; \mathbf{x}'\tau) = \pm \langle \hat{\psi}^\dagger(x', \tau')\, \hat{\psi}(\mathbf{x}, \tau) \rangle = \pm \sum_{\lambda_k < \varepsilon p} \phi_k(\mathbf{x})\, \phi_k(\mathbf{x}') \equiv \pm \rho_0(\mathbf{x}, \mathbf{x}'). \quad (47)$$

On the right-hand side we have introduced the bilocal generalization of the particle density $\rho_0(\mathbf{x})$, which is equal to the diagonal values $\rho_0(\mathbf{x}, \mathbf{x})$.

For fermions filling all states up to an energy ε_F, the free energy (42) is now given by the sum of the eigenvalues

$$F^0[G_0] = \tfrac{1}{2} \sum_{\lambda_k < \varepsilon_F} \lambda_k\,. \quad (48)$$

From the appropriate generalization of the first-order free energy (22), we obtain in analogy to (23) the self-consistent equation for the self-energy

$$\Sigma(\mathbf{x}, \tau; \mathbf{x}', \tau') = \delta(\tau - \tau')\, \delta^{(3)}(\mathbf{x} - \mathbf{x}') \int d^3x'\, V_2(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x}') - V_2(\mathbf{x} - \mathbf{x}')\, \rho(\mathbf{x} - \mathbf{x}') \quad (49)$$

$$\equiv \delta(\tau - \tau')\, \Sigma(\mathbf{x}, \mathbf{x}').$$

For this self-energy we have to solve the time-independent equation

$$\left[\frac{\hat{\mathbf{p}}^2}{2} + V_1(x) \right] \chi_k(\mathbf{x}) + \int d^3x'\, \Sigma(\mathbf{x}, \mathbf{x}')\, \chi_k(\mathbf{x}') = \lambda_k \chi_k(\mathbf{x}), \quad (50)$$

whose solutions provide us via (47) with a new bilocal particle density $\rho(\mathbf{x}, \mathbf{x}')$, to be used for solving again (50), and so on. For fermions, the Hartree–Fock energy is

$$F_{\mathrm{HF}} = \sum_{\lambda_k < \varepsilon_F} \lambda_{\mathbf{k}} - \tfrac{1}{2} \sum_{\lambda_k, \lambda_k' < \varepsilon_F} \int d^3x\, d^3x' [\chi_k^*(\mathbf{x})\, \chi_k(\mathbf{x})\, V_2(\mathbf{x} - \mathbf{x}')\, \chi_{k'}(\mathbf{x}')\, \chi_{k'}(\mathbf{x}')$$
$$- \chi_k^*(\mathbf{x})\, \chi_k(\mathbf{x}')\, V_2(\mathbf{x} - \mathbf{x}')\, \chi_{k'}^*(\mathbf{x})\, \chi_{k'}(\mathbf{x}')]. \quad (51)$$

With the help of our method, this result can be improved systematically by calculating higher-order diagrams of the graphical expansion (20) and extremizing the free energy in Σ. This will yield a self-energy which starts out like (49) and contains in addition bilocal terms in the time. Such equations are of course much harder to solve than the Hartree–Fock–Bogliubov equations, and the solutions cannot be discussed in general, requiring a separate detailed discussion for each physical system. The important lesson we have learned from the anharmonic oscillator which is also a theory with a quartic interaction energy is that the expansion will converge exponentially fast for all coupling strengths.

If pairing effects are important, we may conveniently work with quasi-real doubled fields [5–8]

$$\varphi = \begin{pmatrix} \psi \\ \psi^* \end{pmatrix}, \qquad \text{with} \quad \bar{\varphi} \equiv c\varphi^\dagger = \varphi, \qquad c = \sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \tag{52}$$

and the free part of the free energy is

$$F^0[G_0] = -\frac{1}{2\beta} \operatorname{Tr} \log[G_0], \tag{53}$$

with

$$G_0^{-1} = \begin{pmatrix} \partial_\tau + \hat{\mathbf{p}}^2/2 + V_1(\mathbf{x}) - \mu & 0 \\ 0 & -\partial_\tau - \hat{\mathbf{p}}^2/2 - V_1(\mathbf{x}) + \mu \end{pmatrix}, \tag{54}$$

where we have allowed for the presence of a chemical potential μ, to study grand-canonical ensembles. This is necessary to observe pairing phenomena, since these do not conserve particle number.

The free energy can again be expanded in powers of g with a graphical expansion as in the case of the complex $x(\tau)$ variables, the resulting free energy being a functional $F[G_0]$. In this we set

$$G_0^{-1} = G^{-1} - \Sigma, \tag{55}$$

with

$$\Sigma = \begin{pmatrix} U + V_1 & \Delta \\ \Delta^\dagger & -U - V_1 \end{pmatrix}. \tag{56}$$

The off-diagonal elements are the bilocal gap functions. The lowest-order approximation is the Hartree–Fock–Bogoliubov approximation.

All self-consistent equations can of course be derived also for time-dependent phenomena at zero temperature. We merely have to work with a real time rather than a euclidean one, and calculate the trace of the logarithm in Eqs. (3), (42), (53) for bilocal time-dependent Green functions, with real times in the self-energy equations (23), (49), and in an obvious extensions of the latter to systems with pairing, in which case the above framework provides us with time-dependent Hartree–Fock–Bogoliubov equations.

For large-amplitude collective excitations, the solutions are found most simply since such phenomena require only a semiclassic treatment of the above equations. For any periodic state one chooses some initial self-energy Σ and solves the eigenvalue equation

$$(iG_0^{-1} - \Sigma)\, \chi_k(t) = \lambda_k \chi_k(t), \tag{57}$$

where $\chi_k(t)$ are antiperiodic wave functions whose Fourier decomposition contains only the Matsubara-like frequencies $\omega_n = (2n+1)\pi/T$ and λ_k, the corresponding Bloch–Floquet indices. Then one determines [5, 6]

$$G(t,t') = \sum_k \sum_n \frac{i}{\omega_n - \lambda_k} \exp[-i\omega_n(t-t')]\,\chi_k(t)\,\chi_k(t')$$

$$= \sum_k \frac{1}{\exp(i\lambda_k T)+1} \exp[-i\lambda_k(t-t')]\,\chi_k(t)\,\chi_k(t'), \tag{58}$$

the sum over ω_n producing a Fermi-like distribution containing the period T of oscillations like an imaginary inverse temperature. This Green function (58) is inserted into (57) for a next iteration. The static case follows by taking the limit $T \to \infty$, where the sum reduces to the states below the Fermi surface and $\chi_k(t)$ become time-independent wave functions.

The resulting G can be inserted into the real-time version of the free energy, which is the effective action $\Gamma[G] = -F[G, \Sigma[G]]|_{\beta=-iT}$. A static solution with an infinite period T determines the energy $E[G]$ via the relation $\Gamma[G] = -TE[G]$. For an arbitrary period T, one finds the semiclassical resolvent $R(E) = 1/(H-E)$ by calculating the Fourier transform [9]

$$\int \frac{dT}{2\pi} \exp(i\Gamma[G] + ET) \equiv \frac{\partial W(E)}{\partial E} \exp[iW(E)], \tag{59}$$

where T is the period. Running through the same orbit many times and inserting a phase -1 for each turning point gives

$$R(E) = \frac{\partial W}{\partial E} \sum_{n=1}^{\infty} \exp[inW(E)] = \frac{\partial W}{\partial E} \frac{\exp[iW(E)]}{1+\exp[iW(E)]}, \tag{60}$$

which has pole at $W(E_n) = 2\pi(n+1/2)$ [9].

If an imaginary-time solution passes through a potential barrier, $\exp(-TE) = \exp\{i\Gamma[G]\}$ gives the amplitude of penetration [10].

IV. GRAPHICAL COMPARISON WITH HIGHER EFFECTIVE ACTION VARIATIONAL APPROACH

It is useful to compare our new procedure with the earlier systematic extension of the Hartree–Fock–Bogoliubov approximation [5–7] based on the method of bilocal Legendre transformations. We shall demonstrate in the next section that, although that earlier method is quite appealing, it does not carry to higher orders the most important virtue of the Hartree–Fock–Bogoliubov approximation, the uniform validity for all coupling strengths, including the strong-coupling limit.

Because of the historic significance of the Legendre transformation method, we shall exhibit the precise relation between that and our new procedure.

Legendre transformations provide us with an effective action functional $\Gamma[G]$, whose extrema yield the bilocal density matrix G of the interacting quantum system [11, 12]. Effective actions are an important theoretical tool for formulating extremality principles in quantum field theory and statistical mechanics [13], and their history goes back to the extremality principles of Lee and Yang [11]. They were generalized to bilocal variables by de Dominicis, Martin, and others [12]. The functional $\Gamma[G]$ is specified in terms of a graphical expansion according to the number of fermion loops. We sketch this formalism in real time, where then the lowest contributions lead directly to the time-dependent Hartree–Fock–Bogoliubov equations. Higher corrections are found from a graphical iteration procedure.

To be specific, consider a fermion system. The starting point is an action of the form (41) with an arbitrary two-body force. This will be written in terms of the quasi-real doubled field (52) as

$$\mathscr{A}[\varphi] = \frac{1}{2}\,\varphi G_0^{-1}\varphi - \frac{1}{4!}\,v\varphi\varphi\varphi\varphi, \tag{61}$$

with G_0^{-1} being now c times the matrix G_0^{-1} of Eq. (54). More explicitly, the matrix elements of G_0 contain the free correlation functions

$$G(\mathbf{x}, t; \mathbf{x}', t') \equiv \begin{pmatrix} \langle T_t\, \psi_\alpha(\mathbf{x}, t)\, \psi_\beta(\mathbf{x}', t')\rangle_0 & \langle T_t\, \psi_\alpha(\mathbf{x}, t)\, \psi_\beta^\dagger(\mathbf{x}', t')\rangle_0 \\ \langle T_t\, \psi_\alpha^\dagger(\mathbf{x}, t)\, \psi_\beta(\mathbf{x}', t')\rangle_0 & \langle T_t\, \psi_\alpha^\dagger(\mathbf{x}, t)\, \psi_\beta^\dagger(\mathbf{x}', t')\rangle_0 \end{pmatrix}, \tag{62}$$

where α, β are spin indices, all being suppressed in (61) and the subsequent formulas.

To the action (61) we add a bilocal source term and form the generating functional

$$Z[K] \equiv \int \mathscr{D}\varphi\, \exp\{i[\mathscr{A}[\varphi] + \tfrac{1}{2}\varphi K\varphi]\}, \tag{63}$$

where

$$K \equiv c \begin{pmatrix} \kappa & \lambda \\ \lambda^\dagger & -\kappa^T \end{pmatrix},$$

and $\varphi K\varphi$ is short for $\int dt\, dt'\, \varphi_a(t)\, K_{ab}(t, t')\, \varphi_b(t')$. The superscript T denotes functional transposition, i.e. if spin indices are displayed: $K_{ab}^T(t, t') = K_{ba}(t', t)$, $\mu_{\alpha\beta}^T(t, t') = \mu_{\beta\alpha}(t', t)$. Note that the potential v with four doubled indices is antisymmetric.

Formally, $Z[K]$ can be calculated by removing the interacting part from the integral via functional derivatives, writing

$$Z[K] = \exp\left(-\frac{i}{6}\, v\, \frac{\delta}{i\,\delta K}\, \frac{\delta}{i\,\delta K}\right) Z_0[K], \tag{64}$$

where $Z_0[K]$ is given by a Gaussian functional integral, which can be performed to give

$$Z_0[K] = \int \mathscr{D}\varphi \exp\left[\frac{i}{2}\,\varphi i G_K^{-1}\varphi\right] = \exp\left[\frac{1}{2}\,\mathrm{Tr}\log iG_K^{-1}\right], \tag{65}$$

with $G_K^{-1} = G_0^{-1} + K$. Obviously, G_K is the Green function of the noninteracting fermions in the presence of an external field K. Expanding Z in powers of v results in the standard diagrammatic rules of perturbation theory. If we form the logarithm generating functional

$$iW[K] = \log Z[K], \tag{66}$$

this contains all connected vacuum graphs built from four-vertices and propagators G_K. Because of the fermion nature of φ these are one-particle-irreducible, they coincide with those in Eq. (10), if we drop there all diagrams with three vertices.

Given $W[K]$, it is easy to find the exact density matrix of the system

$$\frac{1}{2}\,G = \frac{\delta W[K]}{\delta K}. \tag{67}$$

An effective action $\Gamma[G]$ of the system is now introduced as the Legendre transform

$$\Gamma[G] \equiv W[K] - \tfrac{1}{2}\,\mathrm{Tr}(KG)\,|_{K=K[G]} \tag{68}$$

such that (67) implies

$$\frac{\delta\Gamma[G]}{\delta G} = -\frac{1}{2}\,K. \tag{69}$$

At the end, the auxiliary source K is set equal to 0. Then Eq. (69) states that the physical density matrix extremizes $\Gamma[G]$, thus providing us with an extremal principle.

Let us evaluate the lowest contributions explicitly: At the one-loop level we have

$$W^{(1)}[K] = -\frac{i}{2}\,\mathrm{Tr}\log iG_K^{-1} \tag{70}$$

and (67) yields $G = G_K$. Reinserting this into (68), we obtain

$$\Gamma[G] \equiv \Gamma^{(0)}[G] + \Gamma^{(1)}[G] = \frac{i}{2}\,\mathrm{Tr}(G_0^{-1}G) - \frac{i}{2}\,\mathrm{Tr}\log iG^{-1}. \tag{71}$$

The extremum of this is the density matrix of the free fermion system $G = G_0$.

We now add to $W[K]$ the lowest two-loop correction in (10),

$$W^{(2)}[K] = -\tfrac{1}{8} v G_K G_K . \tag{72}$$

Exhibiting upper and lower spin component, as well as other particle indices, this contains again Hartree, Fock, and Bogoliubov contributions, whose explicit spin-up and spin-down configurations with the

$$-\tfrac{1}{24} g_{\alpha\beta\gamma\delta}[(G_K)_{\alpha\downarrow\beta\uparrow}(G_K)_{\gamma\downarrow\delta\uparrow} - (G_K)_{\alpha\downarrow\delta\uparrow}(G_K)_{\gamma\downarrow\beta\uparrow} - (G_K)_{\alpha\downarrow\gamma\downarrow}(G_K)_{\beta\uparrow\delta\uparrow}]. \tag{73}$$

By differentiating $W_2[K] = W^{(0)}[K] + W^{(1)}[K] + W^{(2)}[K]$ with respect to K according to (67), we obtain

$$G = G_K - \frac{i}{2} G_K (v G_K) G_K , \tag{74}$$

which is solved for K by

$$K = iG^{-1} - iG_0^{-1} + \tfrac{1}{2} v G, \tag{75}$$

to be reinserted into $W_2[K]$, yielding via (68)

$$\Gamma^{(2)}[\Gamma] = G = -\tfrac{1}{8} v G G. \tag{76}$$

Extremizing $\Gamma_2[K] = \Gamma^{(0)}[K] + \Gamma^{(1)}[K] + \Gamma^{(2)}[K]$ yields

$$G = i[iG_0^{-1} - \tfrac{1}{2} v G]^{-1}, \tag{77}$$

corresponding to the time-dependent Hartree–Fock–Bogoliubov equation (23).

Let us indicate how the method developed in Refs. [5–7] would proceed to higher-loop approximations. Most efficiently, one would use the obvious functional identity

$$\int D\varphi \, \frac{\delta}{\delta \varphi} \, \varphi \exp\left[i\mathscr{A}[\varphi] + \frac{i}{2} \varphi K \varphi \right] = 0, \tag{78}$$

and work out the differentiations leading to the functional differential equation

$$(iG_0^{-1} + K) W_{,K} + \frac{i}{3} v (W_{,KK} + i W_{,K}^2) - \frac{i}{2} = 0, \tag{79}$$

where subscripts separated by a comma indicate functional differentiation with respect to that variable. Using the relations (67) and $-iW_{,KK}=G_{,K}/2=K^{-1}_{,G}/2=-\Gamma^{-1}_{,GG}/4$, this becomes

$$(iG_0^{-1}-2\Gamma_{,G})G-\frac{1}{3!}\,v(i\Gamma^{-1}_{,GG}+G^2)-i=0. \tag{80}$$

After separating out the trivial part, $\Gamma^{(0)}[G]$ the interacting part of $\Gamma[G]$ is found to satisfy the coupled equations

$$\Gamma^{\rm int}_{,G}[G]\,G=-\frac{1}{4}\,vGG+\frac{i}{12}\,vG^4\alpha, \tag{81}$$

$$\alpha=-4\Gamma^{\rm int}_{,GG}(1-2iGG\Gamma^{\rm int}_{,GG})^{-1}=-4\Gamma^{\rm int}_{,GG}+2i\Gamma^{\rm int}_{,GG}GG\alpha. \tag{82}$$

The quantity α represents the exact four-particle vertex function of the theory. The equation is pictured in Fig. 1. This equation generates precisely those vacuum graphs which do not fall into pieces by cutting two lines, i.e. the two-particle-irreducible diagrams. Up to two loops, we have

$$\Gamma[G]=\equiv\Gamma^{(0)}[G]+\Gamma^{(1)}[G]+\Gamma^{\rm int}[G], \tag{83}$$

with the diagrams

$\Gamma^{\rm int}[G]=$ $\frac{1}{8}$  $-\frac{1}{48}$  $+\frac{1}{48}$  $+\ldots$. (84)

In general, effective action has the expansion

$$\Gamma[\Sigma,G]=-\frac{i}{2}\,{\rm Tr}\log(iG_0^{-1}-\Sigma)-\frac{1}{2}\,{\rm Tr}(G\Sigma)-\frac{1}{8}\,vGG+\sum_{n\geqslant 3}^{\infty}\Gamma^{(n)}[G], \tag{85}$$

with $\Gamma^{(n)}$ collecting all two-particle-irreducible graphs with n loops. The extremality condition $\Gamma_G[G]=0$ produces a Green function

$$G=i\{G_0^{-1}-\Sigma[G]\}^{-1}, \tag{86}$$

with a self-energy improving upon the Hartree–Fock–Bogoliubov approximation (77):

$$\frac{1}{2}\,\Sigma[G]=-\Gamma^{\rm int}_{G}[G]=\frac{1}{4}\,vG-\frac{i}{12}\,vG^3\alpha=\frac{1}{4}\,vG-\sum_{n\geqslant 3}^{\infty}\Gamma^{(n)}_{,G}[G]. \tag{87}$$

Equation (86) was first used by Dyson [13] with the prescription that $\Sigma[G]$ contains all those one-particle-irreducible self-energy graphs. Precisely the same diagrams are included here, since removing one line from all two-particle-irreducible diagrams produces all one-particle-irreducible diagrams. Thus the method of Legendre transforms is the perfect tool to derive Dyson's equation.

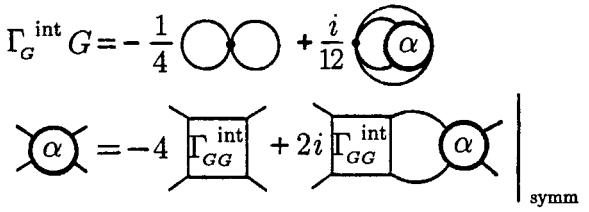


FIG. 1. Recursion relation for two-particle-irreducible graphs in the effective action $\Gamma^{\text{int}}[G]$.

It is a general belief that a set of better and better approximations to the final result can be obtained by calculating all two-particle-irreducible diagrams in $\Gamma[G, \Sigma]$ up to a certain order in the coupling strength and minimizing that expression in G. As we shall see in the next section, however, this belief is disappointed even by the simplest system with a quartic self-interaction, the classical anharmonic oscillator.

From the above diagrammatic analysis, the relation of the Legendre transform method to our systematic extension of the Hartree–Fock–Bogoliubov approximation is now obvious: If the iteration of the new equation (39) for the self-energy is interrupted after the first step (40), we fall back onto the earlier approach. The example in the next section will show that the full iteration of Eq. (39) is essential for the possibility of going to the strong-coupling limit in each approximation.

V. COMPARISON OF CONVERGENCE OF THE TWO SYSTEMATIC EXTENSIONS

To illustrate the improvement brought about by the new systematic extension of the Hartree–Fock–Bogoliubov approximation with respect to the previous higher effective action approach consider the classical partition function of an anharmonic oscillator, which is given by the simple model integral,

$$Z = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi/\beta\omega^2}}\, e^{-\beta(\omega^2 x^2/2 + g x^4/4!)}. \tag{88}$$

It is easy to expand this in powers of g as $Z = \sum_{k=0}^{\infty} z^{(k)} g'^k$, where $g' \equiv g/\beta\omega^4$. The coefficients are

$$z^{(k)} = \frac{(-1)^k}{6^k k!}\, \frac{\Gamma(2k+1/2)}{\Gamma(1/2)}, \qquad k = 0, 1, 2, ..., \tag{89}$$

starting out like $(-)^k$ times 1, $\frac{1}{8}$, $\frac{35}{384}$, $\frac{385}{3072}$, $\frac{25025}{98304}$, $\frac{1616615}{2359296}$, $\frac{260275015}{113246208}$, $\frac{929553625}{100663296}$, $\frac{835668708875}{19327352832}$, ... For large k, they grow like $(-1)^k (2/3)^k k!/k\pi\sqrt{2}$. The series is

divergent, but Borel-summable. It possesses an absolutely convergent strong-coupling expansion in powers of $1/\sqrt{g'}$. This is found by rewriting (88) as

$$Z = (g'/6)^{-1/4} \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{dy}{\sqrt{y}} e^{-y/\sqrt{g'/6}} e^{-y^2} \tag{90}$$

and expanding the first exponential in a Taylor series. The result is the strong-coupling series

$$Z = (g'/6)^{-1/4} \sum_{k=0}^{\infty} \xi_k \left(\frac{1}{\sqrt{g'/6}} \right)^k, \tag{91}$$

with coefficients

$$\xi_k = \frac{1}{2\sqrt{\pi}} (-1)^k \frac{\Gamma(k/2 + 1/4)}{k!}. \tag{92}$$

The series may be expressed in terms of well-known mathematical functions as

$$Z = e^{3/4g'} W_{0,-1/4}(3/2g') = \frac{1}{\sqrt{2\pi}} \left(\frac{3}{g'} \right)^{1/2} e^{3/4g'} K_{1/4}(3/4g'), \tag{93}$$

where $W_{0,-1/4}(z)$ is Whittaker's function and $K_{1/4}(z)$ the modified Bessel function. For $g \to \infty$, Z behaves like a power of g':

$$Z \xrightarrow[g \to \infty]{} \zeta_0 (g'/6)^{-1/4}, \tag{94}$$

with coefficient

$$\zeta_0 = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{dy}{\sqrt{y}} e^{-y^2} = \frac{\Gamma(1/4)}{2\sqrt{\pi}} \approx 1.0227657. \tag{95}$$

The free energy F of the model integral is defined by $Z \equiv e^{-\beta F}$. It has the power series expansion

$$\beta F = \sum_{n=1}^{\infty} f_n \left(\frac{g}{\beta \omega^4} \right)^n \tag{96}$$

with expansion coefficients f_n being equal to $\frac{1}{8}$, $-\frac{1}{12}$, $\frac{11}{96}$, $-\frac{17}{72}$, $\frac{619}{960}$, $-\frac{709}{324}$, $\frac{858437}{96768}$, $-\frac{54193}{1296}$, $\frac{18639247}{82944}$, respectively.

In order to set up our variational approximations to this divergent expansion we observe that the free propagator of the model integral (88) is

$$G_0 \equiv a^2 = \frac{1}{\omega^2} \tag{97}$$

According to Eq. (17), the interacting correlation function G is introduced by replacing

$$G_0 \to (G^{-1} - \Sigma)^{-1} = G + G\Sigma + G\Sigma G. \tag{98}$$

In this model, it will be convenient to express G in terms of a variational frequency Ω by setting the self-energy equal to

$$\Sigma \equiv \Omega^2 - \omega^2. \tag{99}$$

Then the interacting correlation function G becomes simply

$$G = \frac{1}{\Omega^2}, \tag{100}$$

and the replacement rule (98) turns into

$$\omega \to \sqrt{\Omega^2 + \omega^2 - \Omega^2} = \Omega \left[1 + \frac{1}{2} \frac{\omega^2 - \Omega^2}{\Omega^2} - \frac{1}{8} \left(\frac{\omega^2 - \Omega^2}{\Omega^2} \right)^2 - \cdots \right]. \tag{101}$$

The variational approximation βF_N is found by inserting this into the perturbation expansion for βF and re-expanded everything into powers of $\omega^2 - \Omega^2$ up to the order N. For the free part βF^0 of the energy (16), the result is

$$\beta F^0 = \frac{1}{2} \log \frac{\Omega^2}{\omega^2} + \frac{\omega^2 - \Omega^2}{2\Omega^2} - \frac{(\omega^2 - \Omega^2)^2}{4\Omega^4} + \frac{(\omega^2 - \Omega^2)^3}{6\Omega^6} \cdots + \frac{(\omega^2 - \Omega^2)^9}{18\Omega^{18}} + \cdots. \tag{102}$$

Whereas in general, βF is a functional of G and Σ, it reduces in this simple model to a function of Ω. The first three powers in $\omega^2 - \Omega^2$ correspond to the Feynman diagrams (19).

By reexpanding the series (96) in this way, we obtain the successive interaction energies F_N^{int}, with F_3^{int} corresponding to the Feynman diagrams (20):

$$\beta F_1^{\text{int}}(\Omega) = \frac{g}{8\Omega^4},$$

$$\beta F_2^{\text{int}}(\Omega) = g \left(\frac{-1}{4\Omega^6} + \frac{3}{8\Omega^4} \right) - \frac{g^2}{12\Omega^8},$$

$$\beta F_3^{\text{int}}(\Omega) = \frac{11g^3}{96\Omega^{12}} + g^2 \left(\frac{1}{3\Omega^{10}} - \frac{5}{12\Omega^8} \right) + g \left(\frac{3}{8\Omega^8} - \frac{1}{\Omega^6} + \frac{3}{4\Omega^4} \right),$$

$$\begin{aligned} \beta F_4^{\text{int}}(\Omega) = & -\frac{17g^4}{72\Omega^{16}} + g^3 \left(\frac{-11}{16\Omega^{14}} + \frac{77}{96\Omega^{12}} \right) + g^2 \left(\frac{-5}{6\Omega^{12}} + \frac{2}{\Omega^{10}} - \frac{5}{4\Omega^8} \right) \\ & + g \left(\frac{-1}{2\Omega^{10}} + \frac{15}{8\Omega^8} - \frac{5}{2\Omega^6} + \frac{5}{4\Omega^4} \right), \end{aligned}$$

$$\begin{aligned} \beta F_5^{\text{int}}(\Omega) = & \frac{619g^5}{960\Omega^{20}} + g^4 \left(\frac{17}{9\Omega^{18}} - \frac{17}{8\Omega^{16}} \right) + g^3 \left(\frac{77}{32\Omega^{16}} - \frac{11}{2\Omega^{14}} + \frac{77}{24\Omega^{12}} \right) \\ & + g^2 \left(\frac{5}{3\Omega^{14}} - \frac{35}{6\Omega^{12}} + \frac{7}{\Omega^{10}} - \frac{35}{12\Omega^8} \right) + g \left(\frac{5}{8\Omega^{12}} - \frac{3}{\Omega^{10}} + \frac{45}{8\Omega^8} - \frac{5}{\Omega^6} + \frac{15}{8\Omega^4} \right), \end{aligned}$$

$$\beta F_6^{\rm int}(\Omega) = -\frac{709g^6}{324\Omega^{24}} + g^5\left(\frac{-619}{96\Omega^{22}} + \frac{6809}{960\Omega^{20}}\right) + g^4\left(\frac{-17}{2\Omega^{20}} + \frac{170}{9\Omega^{18}} - \frac{85}{8\Omega^{16}}\right)$$
$$+ g^3\left(\frac{-77}{12\Omega^{18}} + \frac{693}{32\Omega^{16}} - \frac{99}{4\Omega^{14}} + \frac{77}{8\Omega^{12}}\right)$$
$$+ g^2\left(\frac{-35}{12\Omega^{16}} + \frac{40}{3\Omega^{14}} - \frac{70}{3\Omega^{12}} + \frac{56}{3\Omega^{10}} - \frac{35}{6\Omega^8}\right)$$
$$+ g\left(\frac{-3}{4\Omega^{14}} + \frac{35}{8\Omega^{12}} - \frac{21}{2\Omega^{10}} + \frac{105}{8\Omega^8} - \frac{35}{4\Omega^6} + \frac{21}{8\Omega^4}\right),$$

$$\beta F_7^{\rm int}(\Omega) = \frac{858437g^7}{96768\Omega^{28}} + g^6\left(\frac{709}{27\Omega^{26}} - \frac{9217}{324\Omega^{24}}\right) + g^5\left(\frac{6809}{192\Omega^{24}} - \frac{619}{8\Omega^{22}} + \frac{6809}{160\Omega^{20}}\right)$$
$$+ g^4\left(\frac{85}{3\Omega^{22}} - \frac{187}{2\Omega^{20}} + \frac{935}{9\Omega^{18}} - \frac{935}{24\Omega^{16}}\right)$$
$$+ g^3\left(\frac{231}{16\Omega^{20}} - \frac{385}{6\Omega^{18}} + \frac{3465}{32\Omega^{16}} - \frac{165}{2\Omega^{14}} + \frac{385}{16\Omega^{12}}\right)$$
$$+ g^2\left(\frac{14}{3\Omega^{18}} - \frac{105}{4\Omega^{16}} + \frac{60}{\Omega^{14}} - \frac{70}{\Omega^{12}} + \frac{42}{\Omega^{10}} - \frac{21}{2\Omega^8}\right)$$
$$+ g\left(\frac{7}{8\Omega^{16}} - \frac{6}{\Omega^{14}} + \frac{35}{2\Omega^{12}} - \frac{28}{\Omega^{10}} + \frac{105}{4\Omega^8} - \frac{14}{\Omega^6} + \frac{7}{2\Omega^4}\right),$$

$$\beta F_8^{\rm int}(\Omega) = -\frac{54193g^8}{1296\Omega^{32}} + g^7\left(\frac{-858437}{6912\Omega^{30}} + \frac{4292185}{32256\Omega^{28}}\right)$$
$$+ g^6\left(\frac{-9217}{54\Omega^{28}} + \frac{9926}{27\Omega^{26}} - \frac{64519}{324\Omega^{24}}\right)$$
$$+ g^5\left(\frac{-6809}{48\Omega^{26}} + \frac{88517}{192\Omega^{24}} - \frac{8047}{16\Omega^{22}} + \frac{88517}{480\Omega^{20}}\right)$$
$$+ g^4\left(\frac{-935}{12\Omega^{24}} + \frac{340}{\Omega^{22}} - \frac{561}{\Omega^{20}} + \frac{3740}{9\Omega^{18}} - \frac{935}{8\Omega^{16}}\right)$$
$$+ g^3\left(\frac{-231}{8\Omega^{22}} + \frac{2541}{16\Omega^{20}} - \frac{4235}{12\Omega^{18}} + \frac{12705}{32\Omega^{16}} - \frac{1815}{8\Omega^{14}} + \frac{847}{16\Omega^{12}}\right)$$
$$+ g^2\left(\frac{-7}{\Omega^{20}} + \frac{140}{3\Omega^{18}} - \frac{525}{4\Omega^{16}} + \frac{200}{\Omega^{14}} - \frac{175}{\Omega^{12}} + \frac{84}{\Omega^{10}} - \frac{35}{2\Omega^8}\right)$$
$$+ g\left(-\frac{1}{\Omega^{18}} + \frac{63}{8\Omega^{16}} - \frac{27}{\Omega^{14}} + \frac{105}{2\Omega^{12}} - \frac{63}{\Omega^{10}} + \frac{189}{4\Omega^8} - \frac{21}{\Omega^6} + \frac{9}{2\Omega^4}\right),$$

$$\beta F_9^{\text{int}}(\Omega) = \frac{18639247 g^9}{82944\Omega^{36}} + g^8\left(\frac{54193}{81\Omega^{34}} - \frac{921281}{1296\Omega^{32}}\right)$$
$$+ g^7\left(\frac{4292185}{4608\Omega^{32}} - \frac{858437}{432\Omega^{30}} + \frac{4292185}{4032\Omega^{28}}\right)$$
$$+ g^6\left(\frac{64519}{81\Omega^{30}} - \frac{46085}{18\Omega^{28}} + \frac{24815}{9\Omega^{26}} - \frac{322595}{324\Omega^{24}}\right)$$
$$+ g^5\left(\frac{88517}{192\Omega^{28}} - \frac{47663}{24\Omega^{26}} + \frac{619619}{192\Omega^{24}} - \frac{56329}{24\Omega^{22}} + \frac{619619}{960\Omega^{20}}\right)$$
$$+ g^4\left(\frac{187}{\Omega^{26}} - \frac{12155}{12\Omega^{24}} + \frac{2210}{\Omega^{22}} - \frac{2431}{\Omega^{20}} + \frac{12155}{9\Omega^{18}} - \frac{2431}{8\Omega^{16}}\right)$$
$$+ g^3\left(\frac{847}{16\Omega^{24}} - \frac{693}{2\Omega^{22}} + \frac{7623}{8\Omega^{20}} - \frac{4235}{3\Omega^{18}} + \frac{38115}{32\Omega^{16}} - \frac{1089}{2\Omega^{14}} + \frac{847}{8\Omega^{12}}\right)$$
$$+ g^2\left(\frac{10}{\Omega^{22}} - \frac{77}{\Omega^{20}} + \frac{770}{3\Omega^{18}} - \frac{1925}{4\Omega^{16}} + \frac{550}{\Omega^{14}} - \frac{385}{\Omega^{12}} + \frac{154}{\Omega^{10}} - \frac{55}{2\Omega^8}\right)$$
$$+ g\left(\frac{9}{8\Omega^{20}} - \frac{10}{\Omega^{18}} + \frac{315}{8\Omega^{16}} - \frac{90}{\Omega^{14}} + \frac{525}{4\Omega^{12}} - \frac{126}{\Omega^{10}} + \frac{315}{4\Omega^8} - \frac{30}{\Omega^6} + \frac{45}{8\Omega^4}\right). \quad (103)$$

For brevity, we have set β and ω equal to 1 on the right-hand sides.

By extremizing $\beta F_N = \beta F^0 + F_N^{\text{int}}$ for $N = 1, 2, 3, ..., 9$, we obtain the free energies as functions of g shown in Fig. 2. We see that the convergence is quite fast. In addition,

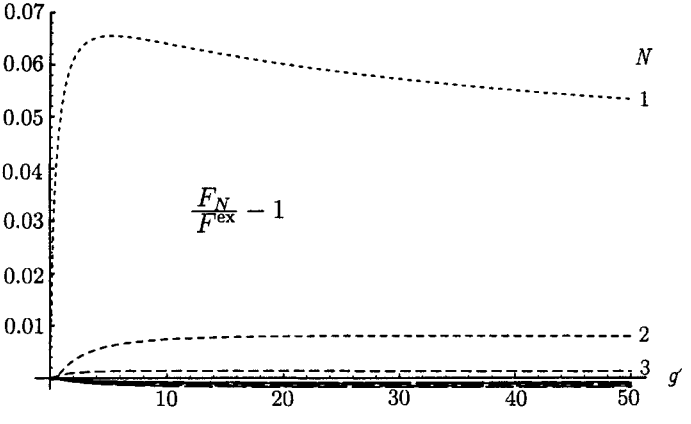


FIG. 2. Relative deviations of the approximate free energies βF_N from the exact free energy βF^{ex} as a function of the dimensionless coupling constant $g' = g/\beta\omega^4$. The length of the dashes is proportional to the order N. The deviations saturate at large g' implying a uniform convergence.

it is uniform up to infinite coupling strength. To exhibit this most clearly, we observe that for increasing $g' = g/\beta\Omega^4$ the optimal value of Ω grows like

$$\frac{\Omega^2}{\omega^2} \sim c \left(\frac{g'}{6}\right)^{1/2}, \tag{104}$$

and the associated free energy like

$$\beta F_N \sim \frac{1}{4} \log\left(\frac{g'}{6}\right) + \beta \hat{F}_N(c), \tag{105}$$

where $\beta \hat{F}_N$ depends on the growth parameter c as

$$\beta \hat{F}_N = \tfrac{1}{2} \log c + \sum_{n=0}^{N} h_n^N c^{-2n},$$

with coefficients listed in Table I.

For $N = 1$ we obtain the Hartree–Fock–Bogoliubov approximation whose particular strength is to give a good approximation to the strong-coupling behaviour $g \to \infty$ of a system. In our model

$$\beta F_1 = \frac{1}{4} \log\left(\frac{g'}{6}\right) - \frac{1}{2} + \frac{1}{2} \log c + \frac{3}{4c^2}. \tag{107}$$

The minimum of this lies at $c = \sqrt{3}$, where $\beta \hat{F}_1 = -\frac{1}{4} + \frac{1}{2} \log \sqrt{3} = 0.02465\ldots$. For the partition function $Z = e^{-\beta F}$, this implies a first approximation $Z_1 \to e^{1/4}/3^{1/4}(g/6)^{1/4}$. The value $e^{1/4}/3^{1/4} \approx 0.9756$ compares reasonably well with the exact value $\zeta_0 = 1.0227657\ldots$ in (95).

TABLE I

Coefficients h_a^N of Reduced Free Energy $\beta \hat{F}_N(c)$ in the Strong-Coupling Expansion (106)

N	0	1	2	3	4	5	6	7	8	9
1	$-\frac{1}{2}$	$\frac{3}{4}$								
2	$-\frac{3}{4}$	$\frac{9}{4}$	-3							
3	$-\frac{11}{12}$	$\frac{9}{2}$	-15	$\frac{99}{4}$						
4	$-\frac{25}{24}$	$\frac{15}{2}$	-45	$\frac{693}{4}$	-306					
5	$-\frac{137}{120}$	$\frac{45}{4}$	-105	693	-2754	$\frac{50139}{10}$				
6	$-\frac{49}{40}$	$\frac{63}{4}$	-210	2079	-13770	$\frac{551529}{10}$	-102096			
7	$-\frac{363}{280}$	21	-378	$\frac{10395}{2}$	-50490	$\frac{1654587}{5}$	-1327248	$\frac{69533397}{28}$		
8	$-\frac{761}{560}$	27	-630	$\frac{22869}{2}$	-151470	$\frac{7169877}{5}$	-9290736	$\frac{1043000955}{28}$	-70234128	
9	$-\frac{7129}{5040}$	$\frac{135}{4}$	-990	22869	-393822	$\frac{50189139}{10}$	-46453680	$\frac{2986001510}{7}$	-1193980176	$\frac{4529337021}{2}$

The reduced free energies $\beta\hat{F}_N$ are plotted in Fig. 3. Their lowest extrema provide us with rapidly convergent approximations to the number (recall (95))

$$\beta\hat{F}_\infty = -\log\zeta_0 = -0.02252\ldots. \tag{108}$$

The approximations $\beta\hat{F}_N$ have for $N=1, 2, 3, \ldots, 9$, the values 0.02465, -0.01311, -0.02136, -0.023759, -0.02386, -0.02291, -0.02265, -0.02253, $-0.02248, \ldots$. The approach is exponentially fast, with oscillations around the correct result (108) (just as those observed for the quantum-mechanical anharmonic oscillator in Ref. [4]). This is illustrated in Fig. 4.

Let us compare this convergent approach with the earlier improvement scheme based on the truncated effective action derived from a Legendre transform [14]. According to Eq. (85), the effective actions to be extremized are

$$\Gamma_N(\Omega) = \frac{1}{2}\log\frac{\Omega^2}{\omega^2} + \frac{\omega^2-\Omega^2}{2\Omega^2} + \sum_{n=1}^{N}(-)^n c_n (g/\beta\Omega^4)^n, \tag{109}$$

where the coefficients c_n require evaluation of all two-particle-irreducible diagrams in the expansion (20), i.e. the Feynman diagrams (84). Because of the simplicity of the model, all Wick contractions with a given number of loops yield the same result, $(g/\beta\omega)^n$, so that the coefficients c_n become simply the multiplicity factors in the diagrammatic expansion (84). For the first three coefficients c_1, c_2, c_3 we therefore obtain directly the numbers $\frac{1}{8}$, $\frac{1}{48}$, $\frac{1}{48}$. All higher coefficients c_n can easily be calculated from a recursion relation derived in Eqs. (101) and (102) of Ref. [6],

$$c_n = \frac{1}{2n}\left[-\frac{1}{6}c_{n-1}(2n-2)(2n-3) + 8\sum_{m=1}^{n-1}(n-m)\,m(2m-1)\,c_m c_{n-m}\right], \tag{110}$$

to be iterated with the initial values $c_1 = 1/8$, $c_2 = 1/48$. This yields for c_3, c_4, ... the sequence $\frac{1}{48}$, $\frac{5}{128}$, $\frac{101}{960}$, $\frac{93}{256}$, $\frac{8143}{5376}$, $\frac{271217}{36864}$, $\frac{374755}{9216}$, ...

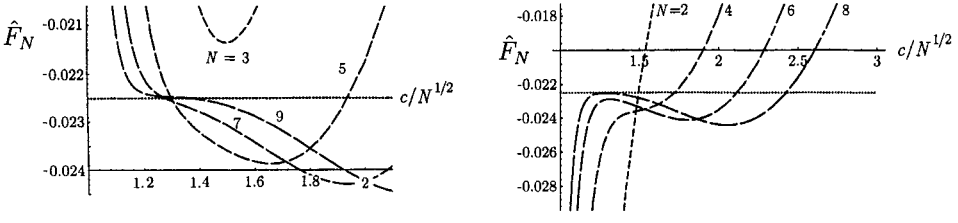


FIG. 3. Reduced free energies $\beta\hat{F}_N$ of Eq. (107) as functions of the growth parameter c. The lowest extrema converge rapidly against the exact strong-coupling value $\log\zeta_0 = -0.02252$—indicated by the horizontal dotted line. For $N=2$ and 4, the turning points yield the approximations $\hat{F}_2$ and $\hat{F}_4$. We have omitted the curve for the Hartree–Fock case $N=1$ which looks similar to the $N=3$-curve but lies much higher, with a minimum at *positive* 0.02465.

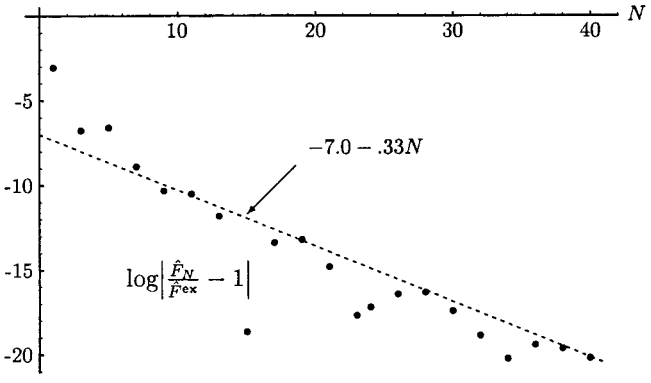


FIG. 4. Exponentially fast convergence of the free energy in the strong-coupling limit. The plot shows the logarithm of the relative error of the Nth approximation as a function of N, which falls off linearly. The approach to the correct result (108) is oscillatory.

In order to cross check the coefficients c_n, we make a power series ansatz $\Omega = \omega[1 + \sum_{n=1}^{\infty} o_n (g/\beta\omega^4)^n]$, insert it into (110), re-expand everything in powers of g, and determine the coefficients o_n to minimize $\Gamma(\Omega)$. This yields $o_n = \frac{1}{4}, -\frac{23}{96}, \frac{61}{128}, -\frac{24805}{18432}, \frac{39247}{8192}, -\frac{35991587}{1769472}, \frac{706267831}{7077888}, -\frac{13947541207}{25165824}, \frac{3112285332185}{905969664}, \ldots$. The resulting series $\Gamma = \sum_{n=1}^{\infty} \gamma_n (g/\beta\omega^4)^n$ turns out to coincide with the original expansion (96) for βF.

The successive approximations of Nth order are plotted in Fig. 5. We observe that the gain in accuracy is not uniform in the coupling strength. Instead, the errors grow rapidly with increasing g. The weakness of this earlier approximation is most dramatic in the limit of infinite coupling strength. Performing the same $g \to \infty$-limit of Ω^2 as in (104), we obtain in analogy to (105) and (106)

$$\Gamma_N = \frac{1}{4} \log\left(\frac{g'}{6}\right) + \Gamma_N(c), \tag{111}$$

with the reduced effective action

$$\Gamma_N = \tfrac{1}{2} \log c + \sum_{n=0}^{N} h_n c^{-2c}, \tag{112}$$

where h_n are equal to $(-)^{n+1}$ times $\frac{1}{2}, \frac{3}{4}, \frac{3}{4}, \frac{9}{2}, \frac{405}{8}, \frac{8181}{10}, \frac{67797}{4}, \frac{5936247}{14}, \frac{197717193}{16}, \frac{819589185}{2}$. Note that, in contrast to our new approximations (106), the expansion coefficients h_n are *independent* of the order N [which is the basic reason why (112) cannot compete with (106)].

For $N = 1$, we obtain the same Hartree–Fock–Boglojubov approximation (107) as in the new approach. However, when attempting to extremize the higher approximations, we find that an extremum exists only for odd orders N, implying that the even approximations $\Gamma_N(\Omega)$ do not possess an extremum for large coupling

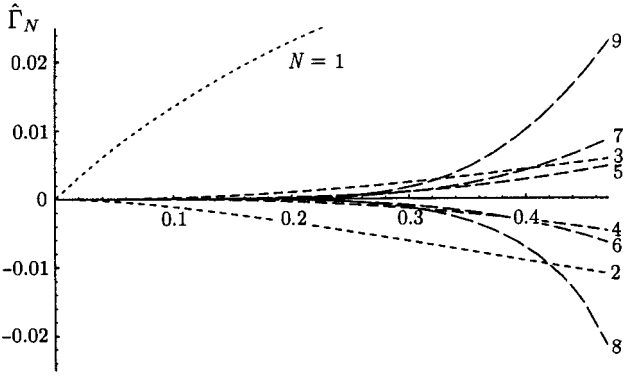


FIG. 5. Approximations to Γ_N to βF obtained from the extrema of the effective action $\Gamma_N(\Omega)$ in Eq. (109) with increasing loop number N. In contrast to the new approximations βF_N in Fig. 2, the errors increase rapidly with increasing g. There is no uniform convergence.

strengths. This can be seen in Fig. 6. Moreover, the limiting values obtained from the odd approximations Γ_N do *not* converge toward the correct limiting value $\beta\hat{F}_\infty = \hat{\Gamma}_\infty = -\log\zeta_0 = -0.02252\ldots$. Instead, they have for $N=1, 3, 5, 7, 9$ the values (see Fig. 6)

$$\Gamma_N = 0.0247,\ 0.0549,\ 0.1187,\ 0.1757,\ 0.2229, \tag{113}$$

which move away from the correct value $-0.02252\ldots$. Thus we conclude that for infinite coupling strengths the previous approximation method based on Legendre transforms is useless beyond the Hartree–Fock–Bogoliubov approximation. Only for very small couplings do higher orders provide us with improved results, as illustrated in Fig. 5.

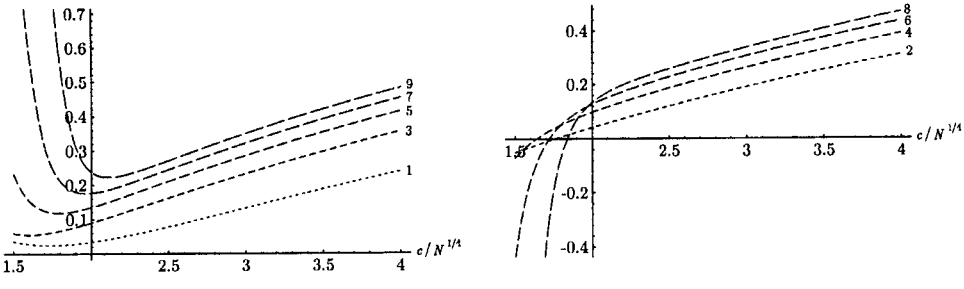


FIG. 6. Reduced effective actions $\hat{\Gamma}_N$ of Eq. (112) as functions of the growth parameter c, with respect to which we must find the minima. Those of the odd-N approximations are all positive and move further and further away from the exact strong-coupling parameter $\log\zeta_0 = -0.02252$. The even-N approximations have neither a minimum nor a turning point, indicating that the effective actions for $N>1$ are useless in the strong-coupling limit.

VI. CONCLUSION

We have presented a new systematic extension to the Hartree–Fock–Bogoliubov approximation which is far superior to an older method based on a bilocal version of the loop expansion of the effective action of the second type. The older method which corresponds to solving Dyson's equation with a self-energy consisting of all two-particle-irreducible diagrams up to a given number of loops fails at larger couplings. In contrast, the new method shows an exponentially fast convergence uniformly for all g, including the strong-coupling limit.

While this paper was being refereed, the new method has been successfully used to find the strong-coupling behavior of a scalar $\phi^4(x)$ quantum field theory, and the critical exponents of the theory for all $O(n)$ universality classes [15].

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