PHYSICAL REVIEW A VOLUME 44, NUMBER 4 15 AUGUST 1991

Effective potential for quantum correlation functions

A. Cuccoli and V. Tognetti
Dipartimento di Fisica dell'Università di Firenze, 50125 Firenze, Italy

R. Vaia
Istituto di Elettronica Quantistica del Consiglio Nazionale delle Ricerche, 50127 Firenze, Italy

(Received 21 December 1990)

A method for calculating quantum averages and static correlation functions of configurational observables is introduced, by extending a variational method, which permits the reduction of the problem to the computation of classical-like averages. This approach opens the possibility of obtaining novel results in many fields, and strongly shortens the computer time needed for numerical calculations. As an example, the well-known sine-Gordon model is considered, and its relevant quantum correlation functions are calculated on the whole temperature range.

In recent years growing interest has been devoted to the statistical mechanics of quantum physical systems with strong nonlinear interactions. The value of methods that allow the reduction of the quantum calculations to classical ones, through the introduction of suitable effective potentials, is therefore apparent.

The best known procedures to obtain effective classical potentials, introduced by Wigner [1] and Feynman [2], undergo serious shortcomings when applied to solids. In fact, the first one is essentially based on an expansion of the quantum statistical distribution function in powers of $\hbar$ and $\beta = T^{-1}$, and therefore it rapidly becomes unreliable at low temperatures. On the other hand, Feynman's original approach defines an effective potential for the free energy, starting from the free-particle propagator, which is definitely not a good approximation for the bound particles in a solid.

Recently a strong improvement of Feynman's variational method [3–5] has been obtained using a quadratic trial action. In such a way the quantum behavior of the harmonic excitations of the system and the classical behavior of the anharmonic part of the potential are fully taken into account in a self-consistent way, so that the thermodynamic properties of solids at high and low temperatures are exactly reproduced, while the quantum anharmonic contributions are also taken into account in a one-loop (Gaussian) approximation. The method gives excellent results for the quantum thermodynamics of chains with both local and nonlocal nonlinear potentials [6–8], and very recently it was found quite useful also in the case of rare-gas solids [9].

The effective potential defined in the previous works has a global character and therefore it is not suitable to obtain statistical averages of configuration-dependent functions like the correlations. A correct variational approximation of the (configurational) density, able to take into account the "local" quantum effects of the interaction, must therefore be introduced; this was previously done only for single-particle interactions [10,11].

In the case of many-body systems, we introduce here an explicit way to evaluate quantum statistical averages of any function of coordinates by means of classical-like configurational integrals, and in particular static correlation functions. Finally, we give explicit results for the quantum correlation functions of the well-known sine-Gordon model.

Let us consider a quantum physical system with coordinates $\hat{q} = \{\hat{q}_1, \ldots, \hat{q}_N\}$ and Hamiltonian $\hat{\mathcal{H}}$. Its partition function is $Z \equiv \exp(-\beta F) = \int dx\, \rho(x)$, where $\rho(x) = \langle x | e^{-\beta\hat{\mathcal{H}}} | x \rangle$ is the (configurational) statistical density at the temperature T, and F is the free energy. The quantum statistical average of a configuration-dependent observable $\hat{C} = C(\hat{q})$ is given by $\langle \hat{C} \rangle = Z^{-1} \int dx\, C(x) \rho(x)$.

Within Feynman's path-integral formulation of quantum statistical mechanics, the density is expressed by the following integral:

$$\rho(x) = \int_x^x \mathcal{D}(\{q_i(u)\}) \times \exp\left[-\frac{1}{\hbar} \int_0^{\beta\hbar} du \left[\sum_{i=1}^{N} \frac{m}{2} \dot{q}_i^2(u) + V(\{q_i(u)\}) \right] \right], \tag{1}$$

where $\int_x^x$ means that we must sum over all closed paths $q(u)$, $u \in [0, \beta\hbar]$, having as initial and final points $x = \{x_i\}$, i.e., $q(0) = q(\beta\hbar) = x$, and the argument of the exponential is minus the Euclidean action $S[q(u)]$.

Long ago Feynman [2] used the free-particle model as the starting point for a variational method. He introduced a "trial" action $S_0[q(u)]$ containing a parameter function that has to be determined by minimizing the right-hand side of the so-called Feynman-Jensen inequality [12]: $F \le F_0 + T \langle S - S_0 \rangle_0$, where F is the "true" free energy of the system, F_0 is the free energy associated with the trial action S_0, and $\langle \cdot \rangle_0$ is the functional average calculated on the path distribution given by S_0.

However, this approximation cannot account for harmonic interactions, and it turns out to be of use only in the range of temperatures higher than the Debye temperature, where the system behaves almost classically, reproducing the results of the Wigner expansion.

In order to extend the method to very low temperatures, it is necessary to treat the harmonic part of the field in a fully quantum way. With this aim, the variational method was strongly improved, and extended to many degrees of freedom, by Giachetti and one of us [3,4], who assumed the general quadratic trial action:

$$S_0[q(u)]=\frac{1}{\hbar}\int_0^{\beta\hbar}du\left[\sum_i\frac{m}{2}\dot{q}_i^2(u)+w(\bar{q})+\frac{m}{2}[q(u)-\bar{q}]^T\times\omega^2(\bar{q})[q(u)-\bar{q}]\right], \tag{2}$$

where $\bar{q}=\bar{q}[q(u)]$ is the average point of the path. The functional character of $\bar{q}$ makes the trial action nonlocal; i.e., we are looking for the best candidate to approximate S within a very large class of functionals, whose path integrals can still be evaluated analytically, except the integral over $\bar{q}$, which is left over as a configurational integral. For many condensed-matter systems, like quantum solids, where the lowest-temperature state is well approximated in terms of quantum harmonic oscillators, the improvement is apparent. The parameter functions of S_0 are the c number $w(\bar{q})$, already considered by Feynman [2], and the $N\times N$ matrix $\omega^2(\bar{q})=\{\omega_{ij}^2(\bar{q})\}$. The minimization of the right-hand side of the Feynman-Jensen inequality gives

$$w(x)=\langle V(x+U^T\eta)\rangle_H-\frac{m}{2}\sum_k\omega_k^2(x)\alpha_k(x)\ , \tag{3}$$

$$m\omega_k^2(x)\delta_{kl}=\sum_{i,j}U_{ki}(x)\langle\partial_{x_i}\partial_{x_j}V(x+U^T\eta)\rangle_H U_{lj}(x)\ , \tag{4}$$

where $\omega_k^2(x)$ are the N eigenfrequencies of the matrix $\omega^2(x)$, which is diagonalized by the orthogonal matrix $U(x)$, and $\alpha_k(x)$ can be interpreted as the pure quantum fluctuation (i.e., the difference between the quantum and the classical fluctuations) of the "kth normal mode":

$$\alpha_k(x)=\frac{\hbar}{2m\omega_k(x)}\left[\coth f_k(x)-\frac{1}{f_k(x)}\right], \tag{5}$$

with $f_k(x)=\beta\hbar\omega_k(x)/2$. The notation $\langle\cdot\rangle_H$ denotes an x-dependent Gaussian average over the quantum fluctuation variables $\eta=\{\eta_k\}$, defined by the moments

$$\langle\eta_k\rangle_H=0,\ \ \langle\eta_k\eta_l\rangle_H=\alpha_k(x)\delta_{kl}\ . \tag{6}$$

The determination (3) also gives $\langle S-S_0\rangle_0=0$, so that the approximation for F is F_0 itself, and this eventually makes it possible to define the "global" effective potential $V_G(x)$ [3,4], by means of which the quantum free energy is expressed in classical-like form:

$$V_G(x)=w(x)+\frac{1}{\beta}\sum_k\ln\frac{\sinh f_k(x)}{f_k(x)}\ . \tag{7}$$

Using the trial action (2), the density $\rho(x)$ can be analytically evaluated [10] in terms of $V_G(x)$.

The final result for a many-body system turns out to be

$$\rho(x)=\left[\frac{m}{2\pi\hbar^2\beta}\right]^{N/2}\int e^{-\beta V_G(x+U^T\eta)}\times\prod_k\frac{d\eta_k}{[2\pi\alpha_k(x+U^T\eta)]^{1/2}}\times\exp\left[-\frac{\eta_k^2}{2\alpha_k(x+U^T\eta)}\right]. \tag{8}$$

The following remarks can be made: (i) a further non-Gaussian smearing (8) is added in respect to the definition of the effective potential; (ii) as already done for the effective potential (7), the expression for $\rho(x)$ can be compared with the results of the Wigner expansion [13], and they agree up to terms of order $\hbar^2$ and β^3 [14]; (iii) as it is implicit from the choice of the trial action, the result (8) for the density is exact if the potential V is purely quadratic.

We present here very useful expressions obtained by using Eq. (8) to calculate quantum averages of configuration-dependent observables $C(\hat{q})$ of systems that are invariant under translations by a lattice vector and under inversion of coordinates. For the sake of simplicity, we consider the case of a one-dimensional lattice of particles having only one degree of freedom per site: its generalization to higher-dimensional lattices and more degrees of freedom per particle is straightforward. From (8) we indeed obtain

$$\langle C(\hat{q})\rangle=\langle C(x+U^T\eta)\rangle_{HG}\ , \tag{9}$$

where we have used the shortened notation $\langle\cdot\rangle_G$ for the classical-like configurational averages

$$\langle\cdot\rangle_G=\frac{1}{Z}\left[\frac{m}{2\pi\hbar^2\beta}\right]^{N/2}\int dx(\cdot)e^{-\beta V_G(x)}\ , \tag{10}$$

with the further convention that $\langle\cdot\rangle_{HG}\equiv\langle\langle\cdot\rangle_H\rangle_G$.

For a generic $C(x)$, the average $\langle C(x+U^T\eta)\rangle_H$ can be readily evaluated by expanding $C(x+U^T\eta)$ in power series around the point x, but the remaining average on x is made difficult by the implicit dependence on x of α_k and U. The calculation is highly simplified in the so-called "low-coupling" approximation (LCA), whose meaning and range of validity were discussed in previous works [4,6,8], where it was adopted successfully to obtain the global thermodynamic properties of many-body systems. In fact, in the LCA, the $\omega_k(x)$ can be expanded around their values in the self-consistent minimum configuration x_0 of $V_G(x)$, so that the dependence on x disappears in all quantities but $V_G(x)$, which eventually reads

$$V_G(x)=\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\substack{i_1,\ldots,i_n;\\ j_1,\ldots,j_n}}[V_{i_1j_1\cdots i_nj_n}(x)-nV_{i_1j_1\cdots i_nj_n}(x_0)]\prod_{l=1}^{n}\frac{\alpha_{i_lj_l}}{2}+\frac{1}{\beta}\sum_k \ln\frac{\sinh f_k}{f_k}+O(\hbar^3)\ , \tag{11}$$

where the subscripts denote derivatives with respect to the corresponding components of $x=\{x_i\}$ and $\alpha_{ij}=\sum_k U_{ki}U_{kj}\alpha_k$, α_k and f_k being expressed as in (5) in terms of $\omega_k=\omega_k(x_0)$. Here $U=U(x_0)$, and if the configuration x_0 is translational invariant, $U=\{U_{ki}\}$ turns out to be nothing but a standard real Fourier transform [4], with k running over the first Brillouin zone.

In the LCA the averages $\langle\cdot\rangle_H$ and $\langle\cdot\rangle_G$ can be disentangled, giving

$$\langle C(x)\rangle=\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{i_1,\ldots,i_n}\langle C_{i_1\cdots i_n}(x)\rangle_G\langle\xi_{i_1}\cdots\xi_{i_n}\rangle_H\ , \tag{12}$$

where $\xi_i=\sum_k U_{ki}\eta_k$. The evaluation of quantum averages has therefore been reduced to those ones over the quantum fluctuation variables ξ, which have a Gaussian distribution, and the classical-like ones of $C(x)$ and its derivatives with the effective potential $V_G(x)$. The former averages can be performed analytically, while to the latter all the tools developed for classical systems can be applied.

Simple explicit formulas can be written for correlation functions like $\langle f(x_i)g(x_{i+j})\rangle$:

$$\langle f(x_i)g(x_{i+j})\rangle=\sum_{n,r,s=0}^{\infty}\frac{1}{n!r!s!}\left[\frac{D_0}{2}\right]^{n+r}(D_j)^s\times\langle f^{(2n+s)}(x_i)g^{(2r+s)}(x_{i+j})\rangle_G\ , \tag{13}$$

where

$$D_j=\langle\xi_i\xi_{i+j}\rangle_H=\frac{1}{N}\sum_k\cos(kj)\alpha_k\ . \tag{14}$$

The above outlined method can be usefully applied to the sine-Gordon chain model, described by the Lagrangian

$$\mathcal{L}=Aa\sum_i\left[\frac{\dot\varphi_i^2}{2}-\left[\frac{\Omega_0^2}{2}(\varphi_i-\varphi_{i+1})^2+\Omega_1^2(1-\cos\varphi_i)\right]\right]\ . \tag{15}$$

The energy scale of the nonlinear excitations is settled by the energy of the static kink $E_S=8Aa\Omega_1\Omega_0$, whose length, in units of the lattice spacing a, is $R=\Omega_0/\Omega_1$, and it is convenient to define a reduced dimensionless temperature $t=T/E_S$. The nonlinear quantum character of the system is ruled by the dimensionless coupling parameter $Q=\hbar\Omega_1/E_S$. Note that the reduced temperature scales with E_S, so that in the limit $Q\rightarrow 0$, at fixed and finite t, the classical results are recovered.

The sine-Gordon (SG) system has been extensively studied in the last years because, in the continuum limit ($R\rightarrow\infty$), it is one of the simplest examples of an integrable nonlinear field theory that admits solitary-wave excitations. Moreover, many physical systems can be mapped onto it, as for example the quasi-one-dimensional easy-plane ferromagnet with in-plane Zeeman field [15]. The quantum corrections to the macroscopic thermodynamic properties, like the internal energy and the specific heat, of the SG model have been calculated by the effective-potential method in [4,6,16]. There it is shown that the LCA contains the usual Hartree-Fock approximation for lowest temperatures, and that it is still surely correct also for $t\gg(2\pi)^{-1}Q^2\ln(8R)$, to be compared with the Debye temperature $t_D\simeq QR$, above which the Wigner method begins to hold. The papers cited above contain the explicit expression of the LCA effective potential corresponding to the model (15).

As an application of Eq. (13) to the SG chain, we have calculated the quantum average $\langle\cos\varphi_i\rangle$, and the quantum correlation functions $C_{cc}(j)=\langle\delta\cos\varphi_i\delta\cos\varphi_{i+j}\rangle$ and $C_{ss}(j)=\langle\sin\varphi_i\sin\varphi_{i+j}\rangle$. If the SG equation is taken as a model of a magnetic easy-plane chain, they represent, respectively, the magnetization and the correlation functions of the longitudinal and transverse fluctuations of the magnetization ($\delta\cos\varphi_i=\cos\varphi_i-\langle\cos\varphi_i\rangle$, and $\delta\sin\varphi_i=\sin\varphi_i$, since, by symmetry, $\langle\sin\varphi_i\rangle=0$). For these functions the infinite sums appearing in Eq. (13) can be performed and the result is

$$\langle\cos\varphi_i\rangle=e^{-D_0/2}\langle\cos\varphi_i\rangle_G\ , \tag{16}$$

$$C_{cc}(j)=e^{-D_0}(\cosh D_j\langle\delta\cos\varphi_i\delta\cos\varphi_{i+j}\rangle_G+\sinh D_j\langle\sin\varphi_i\sin\varphi_{i+j}\rangle_G)\ , \tag{17}$$

$$C_{ss}(j)=e^{-D_0}(\sinh D_j\langle\delta\cos\varphi_i\delta\cos\varphi_{i+j}\rangle_G+\cosh D_j\langle\sin\varphi_i\sin\varphi_{i+j}\rangle_G)\ . \tag{18}$$

The explicit calculation of the classical averages $\langle\cdot\rangle_G$ has been performed by using the transfer-integral method. The most significant quantities that better reflect the quantum effects as a function of temperature are not the correlation functions themselves, but are rather the associated correlation lengths, which are therefore reported in the figures.

In Fig. 1 the value of the magnetization $\langle\cos\varphi_i\rangle$ as a function of the temperature is reported for $R=5.4$ and various values of the coupling parameter. The results for the magnetization for $R=10$ and $Q=0.1$ agree with the previous ones [17], obtained by derivation of the free energy.

The quantum correlation functions $C_{cc}(j)$ and $C_{ss}(j)$ show a large increase in their absolute value in comparison with the classical ones for small values of j at low temperature, where the quantum fluctuations are essential, but they decrease more rapidly with the distance j. This is evident from Fig. 2, where the correlation lengths of the fluctuations of the longitudinal and transverse

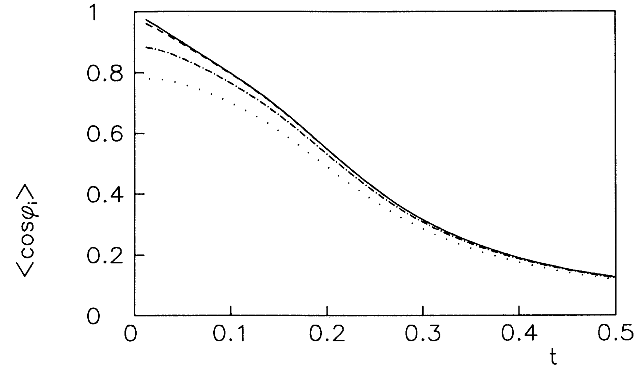

FIG. 1. Temperature dependence of $\langle\cos\varphi\rangle$ for $R=5.4$ and various values of Q. Solid line, classical result; dashed line, quantum result for $Q=0.01$; dash-dotted line, quantum result for $Q=0.05$; dotted line, quantum result for $Q=0.1$.

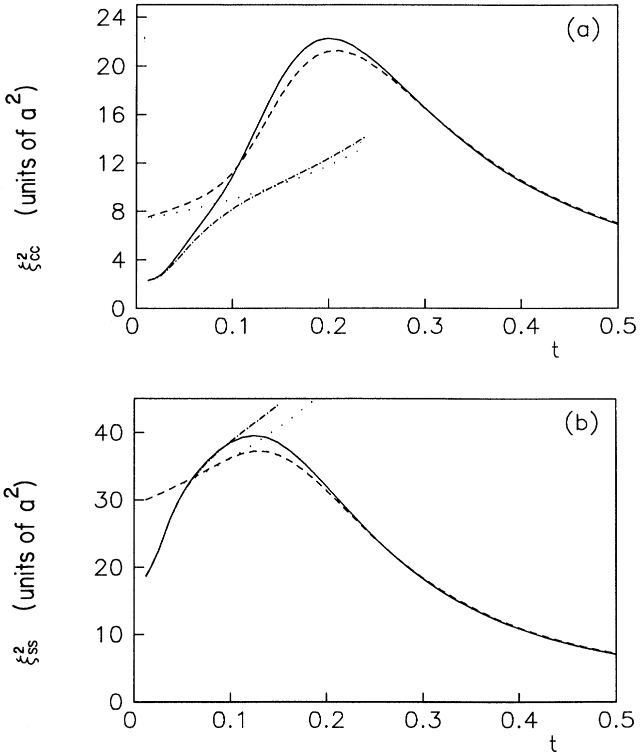

FIG. 2. Temperature dependence of the squared correlation length ξ^2 associated with (a) C_{cc} and (b) C_{ss} for $R=5.4$ and $Q=0.1$. The definition is the usual one: $\xi^2=\sum_j j^2 C(j)/[\sum_j C(j)]$. Solid line, quantum result; dashed line, classical result; dash-dotted line, quantum harmonic approximation; dotted line, classical harmonic approximation.

components of the magnetization are reported together with the corresponding results for the classical sine-Gordon chain. In both cases there is a strong reduction of the correlation length at low temperature, where it correctly approaches the value given by the harmonic approximation, whereas, as expected, at high temperature the classical results are approached. The behavior of the correlation lengths for intermediate temperature shows significant modifications: the position and intensity of the maximum are changed. A physical explanation for such phenomena can be guessed by noting that the presence of the peak is directly related to the thermal excitation of kinks, as it is proven by the fact that the peak position is almost proportional to the static kink energy [18]; the modifications displayed can therefore be related to the quantum renormalization of the kink energy.

The above example has been given to show the power of our approach, which applies regardless to the integrable character of the model system. It has been done for an integrable system in order to offer a possible comparison when exact results derived by another method [19] will be available for the sine-Gordon model. Work is in progress in this direction, together with the application to the dynamical correlations of rare-gas solids.

Useful discussions and contacts with Professor A. A. Maradudin, Professor G. K. Horton, Professor V. E. Korepin, and Professor A. G. Izergin are gratefully acknowledged.

---

[1] E. P. Wigner, Phys. Rev. **40**, 749 (1932).

[2] R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, MA, 1972).

[3] R. Giachetti and V. Tognetti, Phys. Rev. Lett. **55**, 912 (1985).

[4] R. Giachetti and V. Tognetti, Phys. Rev. B **33**, 7647 (1986).

[5] R. P. Feynman and H. Kleinert, Phys. Rev. A **34**, 5080 (1986).

[6] R. Giachetti, V. Tognetti, and R. Vaia, Phys. Rev. A **37**, 2165 (1988).

[7] R. Giachetti, V. Tognetti, and R. Vaia, Phys. Rev. A **38**, 1521 (1988).

[8] A. Cuccoli, V. Tognetti, and R. Vaia, Phys. Rev. B **41**, 9588 (1990).

[9] S. Liu, G. K. Horton, and E. R. Cowley, Phys. Lett. A **152**, 79 (1990).

[10] H. Kleinert, Phys. Lett. A **118**, 267 (1986).

[11] R. Vaia and V. Tognetti, Int. J. Mod. Phys. B **4**, 2005 (1990).

[12] H. Leschke, in *The Path Integral Method with Applications,* edited by A. Ranfagni *et al.* (World Scientific, Singapore, 1988).

[13] G. Nienhuis, J. Math. Phys. **11**, 239 (1970).

[14] H. Janke, in *Path Integrals from meV to Mev,* edited by V. Sa-Yakanit *et al.* (World Scientific, Singapore, 1989).

[15] H. J. Mikeska, J. Phys. C **11**, L29 (1978).

[16] R. Giachetti, V. Tognetti, and R. Vaia, Phys. Rev. A **38**, 1638 (1988).

[17] R. Giachetti, V. Tognetti, and R. Vaia, J. Phys. (Paris) Colloq. **50**, C3-59 (1989).

[18] T. Schneider and E. Stoll, Phys. Rev. B **22**, 5317 (1980).

[19] A. R. Its, A. G. Izergin, V. E. Korepin, and N. A. Slavnov, Int. J. Mod. Phys. B **4**, 303 (1990).