PHYSICAL REVIEW LETTERS

VOLUME 64

8 JANUARY 1990

NUMBER 2

Holomorphic Representation of a Set of Supercoherent Canonical Coordinates for a Quantum Oscillator with x^{2K} Anharmonicity

J. S. Arponen

Department of Theoretical Physics, University of Helsinki, Siltavuorenpenger 20C, 00170 Helsinki, Finland

R. F. Bishop

*Department of Mathematics, University of Manchester, Institute of Science and Technology, P.O. Box 88,
Manchester M60 1QD, England*

(Received 19 June 1989)

The coupled-cluster method is widely applicable to quantum systems of interacting particles or fields. Such concepts as supercoherent states, generalized order parameters, and exact mappings onto corresponding multilocal classical field theories arise naturally within it, particularly in its extended version. Its holomorphic representation is applied here to the anharmonic oscillator, in order to demonstrate several key mathematical features.

PACS numbers: 03.65.Fd, 11.10.Lm, 31.20.Tz, 42.50.Dv

There are many fields in modern theoretical physics where a key role is played by one or more of such related concepts or constructs as multicoherent or supercoherent states, generalized mean fields or generalized order parameters, exact mappings of local quantum field theories onto some multilocal classical counterpart, and techniques which go beyond some appropriate Bogoliubov or Gaussian approximations. The squeezed or two-photon coherent states of considerable current interest in quantum optics,¹ and the various attempts to generalize them to their n -photon counterparts with $n > 2$,² provide a topical example where each of the above concepts has come forcefully into play. Examples also abound in quantum field theory of largely problematic attempts to proceed systematically beyond the Gaussian approximation in, for example, a Feynman path-integral formulation.

It is our intention to show here that the coupled-cluster method (CCM) of quantum many-body theory,^{3,4} particularly its more recent extended (ECCM) version,^{5,6} provides an interesting framework for incorporating and unifying all of the above underlying motifs. As an example, we illustrate it here on the well-studied one-dimensional quantum anharmonic oscillators, con-

sidered as model field theories. These theories are quite singular, because if the number of spatial dimensions is considered to be ≥ 1 , there is an exceptionally large interaction between the zero-momentum modes. We show that the holomorphic representation of the CCM in the appropriate Bargmann space for this model provides not only an extremely stringent test of the method, but also an illustration of how each of the above ideas or concepts may be fully implemented. On the other hand, the model (at least in the quartic case) is very well understood via alternative techniques.⁷

The CCM was introduced in many-body theory to take full advantage of the linked-cluster theorem for systems with normal Schrödinger dynamics. Because of its universality the CCM can be invariably used for arbitrary quantum systems. It has very successfully been applied to a number of many-body problems in nuclear physics, quantum chemistry, condensed matter theory, and others areas.^{4,8,9} Through a parametrization of the Hilbert space in terms of a set of multilocal (m -body, $m = 1, 2, 3, \dots$) field amplitudes the CCM maps the quantum theory into classical Hamiltonian mechanics in a symplectic phase space. In this paper we emphasize such basic mathematical features of the method, particu-

larly the ECCM, as its existence and convergence properties. We remark that such concepts as connectivity and multiple linking of the many-body subsystems and their correlations are normally analyzed diagrammatically. The spirit of the present work is to make the formalism and all such concepts fully algebraic in order to shed further light on them. We know of no other comparable example where the asymptotic analytic behavior of the various amplitudes which completely and exactly characterize the system has been so fully analyzed. In particular, we show that various formally divergent series may be given precise, *but generally nonunique*, interpretations.

The Hamiltonian to be considered is $H = \frac{1}{2}p^2 + V(x)$, where $V(x) = \frac{1}{2}\lambda x^{2K}$ and $K=2,3,\dots$. The eigenvalue equation for the ground-state wave function $\langle x|\psi\rangle \equiv \psi(x)$ is

$$-\frac{1}{2}\psi''(x) + V(x)\psi(x) = E_0\psi(x),$$

and the normalization of $|\psi\rangle$ is chosen such that $\langle 0|\psi\rangle = 1$, where $\psi^0(x) \equiv \langle x|0\rangle$ is the normalized ground-state wave function of the harmonic oscillator, $H^0 = \frac{1}{2}p^2 + \frac{1}{2}x^2$. The canonical boson operators are defined conventionally by $x = (a^\dagger + a)/\sqrt{2}$ and $p = i(a^\dagger - a)/\sqrt{2}$. The Fock-space ground state of H can be given in the configuration-interaction (CI) form,

$$|\psi\rangle = F(a^\dagger)|0\rangle, \quad F(z) = \sum_{n=0}^{\infty} F_n z^n.$$

The intermediate normalization condition implies $F_0 = 1$. The eigenvalue equation is thus

$$H(a^\dagger, a)F(a^\dagger)|0\rangle = E_0F(a^\dagger)|0\rangle. \quad (1)$$

In the Bargmann space the operators are represented by the algebra $a^\dagger \rightarrow z$, $a \rightarrow d/dz$ of the complex variable z . The ground-state eigenvalue equation (1) thus becomes an ordinary differential equation for $F(z)$ in the complex plane. Using the well-known completeness properties of the normalized Glauber coherent states $|z\rangle = \exp(-\frac{1}{2}|z|^2 + za^\dagger)|0\rangle$, it is straightforward to derive the (Fourier-like) mapping

$$F(z) = \pi^{-1/4} e^{-z^2/2} \int_{-\infty}^{\infty} dx e^{\sqrt{2}zx - x^2/2} \psi(x) \quad (2)$$

between an arbitrary wave function $\psi(x)$ and its holomorphic Bargmann form $F(z)$. Also, the scalar product $\langle g^*|h\rangle \equiv \langle 0|g(a)h(a^\dagger)|0\rangle$ of two holomorphic wave functions $|h\rangle = h(a^\dagger)|0\rangle$ and $|g^*\rangle = g^*(a^\dagger)|0\rangle$ can be expressed in the forms

$$\langle g^*|h\rangle = \pi^{-1} \int d^2z e^{-|z|^2} g(z^*)h(z) \quad (3a)$$

$$= g(d/dz)h(z)|_{z=0} \quad (3b)$$

$$= \sum_{n=0}^{\infty} n! g_n h_n. \quad (3c)$$

These definitions are identical if the two states are nor-

malizable, in which case $h(z) \equiv \sum_n h_n z^n$ and $g^*(z) \equiv \sum_n g_n^* z^n$ are both entire functions of order $\rho \leq 2$. However, differences arise if the Hilbert space of normalizable wave functions is extended into a more general linear vector space. This is precisely what is necessitated by the CCM representations of the state vectors.

In the CCM the CI operator is parametrized as

$$F(a^\dagger) = e^{S(a^\dagger)}, \quad S(a^\dagger) = \sum_{n=1}^{\infty} S_n (a^\dagger)^n.$$

If $F(a^\dagger)$ generates the ground state, the coefficients S_n are the Hubbard linked-cluster amplitudes representing the sums of complete sets of connected open-end diagrams for the ground state. We define the biorthonormal average-value functional $\bar{\mathcal{O}} \equiv \langle \mathcal{O} \rangle$ of an arbitrary operator $\mathcal{O} = \mathcal{O}(a^\dagger, a)$ by $\bar{\mathcal{O}} = \langle 0|\bar{F}\mathcal{O}F|0\rangle / \langle 0|\bar{F}F|0\rangle$, which can be written as

$$\bar{\mathcal{O}} = \langle 0|\Omega(a)e^{-S(a^\dagger)}\mathcal{O}e^{S(a^\dagger)}|0\rangle,$$

$$\langle 0|\Omega(a) \equiv \frac{\langle 0|\bar{F}(a)F(a^\dagger)}{\langle 0|\bar{F}(a)F(a^\dagger)|0\rangle}.$$

Here the function $\bar{F}(a) \equiv \sum_{n=0}^{\infty} \bar{F}_n a^n$ generates an arbitrary bra state. If the Hamiltonian is Hermitian, $\bar{F} \equiv F^*$.

The function $\Omega(z) \equiv \sum_{n=0}^{\infty} \Omega_n z^n$, which gives the average values of the powers of the creation operator $a^\dagger$, can be written as

$$\langle e^{za^\dagger} \rangle = \Omega(z) \equiv \exp \tilde{\Sigma}(z). \quad (4)$$

The cumulant function $\tilde{\Sigma}(z) = \sum_{n=1}^{\infty} \tilde{\sigma}_n z^n$ thus has coefficients given by the connected averages $n!\tilde{\sigma}_n = \langle (a^\dagger)^n \rangle_{\text{conn}}$.

Finally, the function $\Sigma(z) \equiv \sum_{n=1}^{\infty} \sigma_n z^n$ is defined by

$$\Sigma(z) = \langle 0|\Omega(a)(e^{za} - 1)S(a^\dagger)|0\rangle. \quad (5)$$

Hence, the coefficients are

$$\sigma_n = (n!)^{-1} \sum_{m=1}^{\infty} m! \Omega_{m-n} S_m. \quad (6)$$

The sets of free variables which now completely and exactly parametrize the problem may therefore be chosen in the three different ways: $\{F_n, \bar{F}_n\}$, $\{S_n, \Omega_n\}$, and $\{\sigma_n, \tilde{\sigma}_n\}$. These ground-state amplitudes define, respectively, the CI, normal CCM (NCCM), and ECCM parametrizations. In each case the parameters are obtained by requiring $\bar{H}$ to be stationary with respect to infinitesimal variations in the respective amplitudes. Each ground-state amplitude may be expressed diagrammatically in terms of generalized tree diagrams representing sums of definite sets of Goldstone diagrams.^{6,10} Their locality and connectivity properties depend crucially on the particular parametrization. In particular, both CCM parametrizations contain only connected diagrams and incorporate the size-extensivity feature which is absent from the CI method. The important cluster property is obeyed by *all* of the amplitudes only in the ECCM,

and it is this feature which enables its amplitudes to be interpreted as generalized mean fields or quasilocal order parameters.⁶ Conversely, the lack of locality in the present model makes it an especially stringent test of the ECCM. Finally, we note that the complete dynamic problem may be similarly formulated in the three methods by introducing an appropriate quantum-mechanical action functional. It has also been pointed out⁶ that the ECCM can be interpreted as a definite supercoherent bosonization scheme in which the Hilbert space is mapped onto the set of coherent states of some fictitious Bose space, and the quantum many-body correlations are mapped into a formally noncorrelated classical mean-field description.

If an operator $\mathcal{O}(a^\dagger, a)$ and the functions $e^{\pm S}$ are now expressed in the Bargmann form, one finds

$$e^{-S(a^\dagger)} \mathcal{O}(a^\dagger, a) e^{S(a^\dagger)} |0\rangle \rightarrow \mathcal{O}\left[z, \frac{d}{dz} + S'(z)\right].$$

Using Eq. (3b), the average-value functional is thus

$$\mathcal{O} = \Omega\left[\frac{d}{dz}\right] \mathcal{O}\left[z, \frac{d}{dz} + S'(z)\right] \Big|_{z=0}.$$

It is useful first to study the analytic properties of the functions $F(z)$, $S(z)$, $\Omega(z)$, and $\Sigma(z)$ at the exact ground-state point and its immediate vicinity.

Writing $F(z) \equiv e^{-z^2/2} f(z)$, the differential equation for f is

$$\left[\frac{d}{dz}\right]^{2K} f(z) = \frac{2^{K+1}}{\lambda} \left[\left[z - \frac{1}{2} \frac{d}{dz}\right]^2 + E_0\right] f(z).$$

Taking into account Eq. (2) and the reality, positivity, and the even parity of the wave function $\psi(x)$, $f(z)$ is an even entire function of z , which is real and positive on the real axis. We use WKB arguments to establish the qualitative properties of $f(z)$. Asymptotically, for large values of $r = |z| \rightarrow \infty$, there are $2K$ qualitatively different solutions,

$$f_{(n)}(z) = \exp[\varepsilon^n a z^\nu], \quad n = -K+1, \dots, K,$$

where $\nu = 1 + 1/K$, $a = \nu^{-1} 2^{\nu/2} \lambda^{-(\nu-1)/2}$, and $\varepsilon = \exp(i\pi/K)$. Since $F(z)$ is normalizable, the product $e^{-|z|^2/2} |F|^2$ is integrable in the complex plane by Eq. (3a). Therefore, on lines parallel to the imaginary axis, one must have (for x, y real), $|f(x+iy)| \rightarrow o(1)$ as $y \rightarrow \pm\infty$. By using this property, and by carefully matching the various WKB branches it is not difficult to show that

$$f(z) \xrightarrow{r \rightarrow \infty} A \exp[a(\pm z)^\nu] \quad (7)$$

for $|\arg(\pm z)| < \pi/2$, respectively. On the imaginary axis, the left and right solutions are of equal magnitude, and the interference generates an infinite sequence of zeros. the zeros z_m of f (and thus of F) are asymptoti-

cally at points $\pm iy_m$, where

$$y_m \xrightarrow{m \rightarrow \infty} \left[\frac{\pi}{a} \sec\left(\frac{\pi}{2K}\right) \right]^{1/\nu} m^{1/\nu}.$$

By making use of Eq. (4) and the Baker-Campbell-Hausdorff theorem for the exponential operator, we find the general expression

$$\Omega(z) = N^{-2} e^{-z^2/4} \int dx e^{xz/\sqrt{2}} \psi^*(x) \psi(x - z/\sqrt{2})$$

for the function $\Omega(z)$, where $N^2 \equiv \int dx |\psi(x)|^2$. Since $V(x)$ is an analytic function of x , the ground-state wave function $\psi(x)$ can be analytically continued to the whole x plane, and shown to be an entire function of order $K+1$. By considering the asymptotic behavior of $\psi(x)$ for $|x| \rightarrow \infty$, one can readily show that Ω is an entire function of z of order $K+1$ with no zeros on the real axis, and with asymptotic behavior

$$\Omega(x) \propto \exp(-b\lambda^{1/2}|x|^{K+1})$$

as $|x| \rightarrow \infty$, where b is a positive constant.

Since $f(x)$ is an entire function of fractional order $1 < \nu < 2$ and satisfies Eq. (7), it can be represented by the Hadamard decomposition

$$f(z) = \prod_m (1 - z/z_m) e^{z/z_m}.$$

The CCM amplitude $S(z)$ therefore develops logarithmic branch points at the zeros of $f(z)$. Hence, it is often more convenient to use its single-valued first derivative

$$S'(z) = -z + \sum_m \left[\frac{1}{z - z_m} + \frac{1}{z_m} \right]. \quad (8)$$

It is clear that the state $S(a^\dagger)|0\rangle$ is not normalizable in the Hilbert space, and expressions such as in Eqs. (5) and (6) must be treated with care. In particular, the sum in Eq. (6) for σ_n can easily be shown to be formally divergent.

Various techniques can be applied to give an interpretation to the divergent sum in Eq. (6). For example, Fourier methods may be applied to the definition (3b) of the scalar product. Alternatively, the Borel resummation method may be applied to definition (3c). Both methods lead to identical results. In the latter case, for example, it is not difficult to show the important relation

$$\langle 0 | g(a) \frac{1}{a^\dagger - c} | 0 \rangle = -\frac{1}{c} \int_0^{\infty} dw e^{-w} g\left(\frac{w}{c}\right)$$

for a class of functions g , where the integration variable w is in the direction of some unit vector $\eta = \exp(i\varphi)$ with $-\pi/2 < \varphi < \pi/2$, chosen so that the integral is convergent. There may be several disjoint sectors where this requirement is fulfilled, in which case the scalar product would not be uniquely defined.

We apply these results to calculate the amplitudes

$$\sigma_n = (n!)^{-1} \langle 0 | \Omega(a) a^{n-1} S'(a^\dagger) | 0 \rangle, \quad (9)$$

where $S'(a^\dagger)$ is represented as in Eq. (8). Taking into account the asymptotic behavior of the function $\Omega(z)$ and the distribution of the poles of $S'(z)$, it may be seen that the amplitudes σ_n and hence the function $\Sigma(z)$ do not have a unique representation. The origin of this multiplicity of solutions lies in the nonlinear decomposition of the original linear problem. Nevertheless, each of these solutions, when formally expanded, leads to precisely the same divergent expansion (6). Such extra physically motivated constraints as the even parity and reality of the ground-state wave function may still be imposed via Eq. (9). In what follows we constrain the discussion to the definite and unique choice of $\Sigma(z)$ that these particular restrictions imply. In terms of the odd function $R(x)$, defined as the distribution

$$R(x) = \delta'(x) - \frac{1}{2} \operatorname{sgn}(x) \sum_m e^{-x^2 m},$$

where $\delta(x)$ is the Dirac delta, the even functions $S(z)$

and $\Sigma(z)$ may then be found via their derivatives as

$$S'(z) = \int_{-\infty}^{\infty} dx R(x) \sinh(xz), \quad (10a)$$

$$\Sigma'(z) = \int_{-\infty}^{\infty} dx \rho(x) \sinh(xz), \quad (10b)$$

where $\rho(x) \equiv R(x)\Omega(x)$. Equation (10a) defines $S(z)$ only in an infinitesimal region around the origin and on the imaginary axis, whence it can be analytically continued. Equation (10b) defines $\Sigma(z)$ as an entire function. The coupled-cluster amplitudes S_n and σ_n are evidently moments of certain appropriate distributions.

In this static CCM formalism, the expectation value of an arbitrary normal-ordered operator may be found from the generating function

$$A(u, v) \equiv \langle e^{ua^\dagger} e^{va} \rangle.$$

By making use of the explicit definitions of the operators Ω and S , we may derive the relation

$$A(u, v) = \langle 0 | \Omega(a+u) \exp \left[\int_0^v dw S'(a^\dagger + w) \right] | 0 \rangle,$$

and thence by expanding the exponential and using the representation of Eq. (10a),

$$A(u, v) = \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^n \left[\int_{-\infty}^{\infty} dx_i \rho(x_i) (e^{ux_i} - 1)/x_i \right] \exp[\tilde{\Sigma}(u + x_1 + \cdots + x_n) - \tilde{\Sigma}(x_1) - \cdots - \tilde{\Sigma}(x_n)].$$

In particular, this equation gives finite closed-form expressions for the expectation values of such multinomial operators in a and $a^\dagger$ as the Hamiltonian of the present model. For a general normal-ordered operator $\mathcal{O}(a^\dagger, a)$ the average value is now given by $\bar{\mathcal{O}} = \mathcal{O}(\partial_u, \partial_v) \times A(u, v)|_{u=v=0}$ as a functional of the functions $\Sigma(x)$ and $\rho(x)$. Furthermore, the expression may formally be expanded and given a diagrammatic representation with very precise linking and connectivity properties, in terms of the amplitudes $\{\sigma_n, \tilde{\sigma}_n\}$. Precise parallels can clearly be drawn with the more well-known linked (L) and double-linked (DL) expansions for the ECCM average-value functions, expressed in the form

$$\bar{\mathcal{O}} = \sum_n \frac{1}{n!} \langle 0 | e^{\tilde{\Sigma}} \{ \mathcal{O} \Sigma^n \}_L | 0 \rangle_{DL},$$

that have been described elsewhere.^{5,6}

We have thus remarkably succeeded fully to make algebraic the abstract topological linking requirements associated with the structure of the vertices of the emerging ECCM tree diagrams. By invoking the stationarity condition for $\bar{H}$ with respect to the variations of $\tilde{\Sigma}(x)$ and $\rho(x)$ one can solve the ground-state correlation amplitudes and their tree-diagram structure. We stress at this point that the form of the generating function for the average values, once derived, is quite general and not restricted just to the case of the anharmonic oscillator.

In conclusion, it is our belief that the algebraic formulation in terms of the holomorphic representation for the (E)CCM will both enable the method itself to be under-

stood at a deeper level, and increase further its domain of applicability to problems in quantum field and many-body theory.

We thank C. Cronström, C. Montonen, and M. Noga for useful comments. The support of the United Kingdom Science and Engineering Research Council (Great Britain) is gratefully acknowledged.

¹D. F. Walls, *Nature (London)* **306**, 141 (1983).

²R. A. Fisher, M. M. Nieto, and V. D. Sandberg, *Phys. Rev. D* **29**, 1107 (1984); C. Gerry and S. Rodrigues, *Phys. Rev. A* **35**, 4440 (1987).

³F. Coester, *Nucl. Phys.* **7**, 421 (1958); F. Coester and H. G. Kümmler, *ibid.* **17**, 477 (1960).

⁴R. F. Bishop and H. G. Kümmler, *Phys. Today* **40**, No. 3, 52 (1987).

⁵J. Arponen, *Ann. Phys. (N.Y.)* **151**, 311 (1983).

⁶J. S. Arponen, R. F. Bishop, and E. Pajanne, *Phys. Rev. A* **36**, 2519 (1987); *ibid.* **36**, 2539 (1987).

⁷C. M. Bender and T. T. Wu, *Phys. Rev.* **184**, 1231 (1969); B. Simon, *Ann. Phys. (N.Y.)* **58**, 76 (1970); A. Voros, *Ann. Inst. Henri Poincaré A* **39**, 211 (1983).

⁸H. G. Kümmler, in *Nucleon-Nucleon Interaction and Nuclear Many-Body Problems*, edited by S. S. Wu and T. T. S. Kuo (World Scientific, Singapore, 1984), p. 46.

⁹J. Noga, S. A. Kucharski, and R. J. Bartlett, *J. Chem. Phys.* **90**, 3399 (1989).

¹⁰J. Arponen, R. F. Bishop, and E. Pajanne, in *Condensed Matter Theories*, edited by P. Vashishta, R. K. Kalia, and R. F. Bishop (Plenum, New York, 1987), Vol. 2, p. 357.