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An exactly soluble model for matter interacting with radiation

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Abstract. A generalised Dicke model including: (i) the spatial variation of the electromagnetic field; and (ii) quantum Debye vibrations of atoms around their equilibrium positions is proposed. It is proved that the free energy per particle for such a model can be calculated in the thermodynamic limit exactly and rigorously.

1. Introduction

Recently Klemm and Zagrebnov (1977, see also Zagrebnov and Klemm 1976) have investigated rigorously a new model for (solid) matter interacting with the quantised radiation field. They took into account the spatial variation of the electromagnetic field in the cavity Λ and simultaneously assumed that the N two-level atoms in Λ make small classical motions $\{\boldsymbol{u}_j\}$ around their equilibrium positions $\{\boldsymbol{l}_j\}$ in the harmonic lattice. The relation of this new model to the similar Dicke-type models of Hepp and Lieb (1973) and Hioe (1973) has been also discussed.

The purpose of our present paper is to show that for this model one can calculate the free energy per atom in the thermodynamic limit in an exact fashion even if the atoms make the quantum vibrations $\{\hat{\boldsymbol{u}}_j\}$ instead of the classical ones.

The definition of the Hamiltonian and some of its properties are given in § 2. In § 3 we study the corresponding partition function and the free energy per particle in the thermodynamic limit $N\to\infty$, $|\Lambda|\to\infty$, $|\Lambda|/N=v$, where $|\Lambda|$ is the volume of the cavity. Some technical results are accumulated in the appendix.

2. The Hamiltonian

To avoid unnecessary complications we shall consider the simplest version of the model with one photon mode $\{\omega_k, \boldsymbol{k}\}$ and one longitudinal phonon mode $\{\Omega_q, \boldsymbol{q}\}$ such that $\boldsymbol{k}=\boldsymbol{q}=\boldsymbol{Q}$, $|\boldsymbol{Q}|=\pi/a$. Here a is the lattice constant in the $\boldsymbol{Q}$-direction (for discussion see Zagrebnov and Klemm 1976, Klemm and Zagrebnov 1977). The generalisations to the case of multi-level atoms, finite number of modes, non-zero value of electromagnetic wave phase ϕ etc may be carried out straightforwardly in the manner of Zagrebnov *et al* (1975), Hepp and Lieb (1973) or Zagrebnov and Klemm (1976).

For a sinusoidal standing electromagnetic wave with $\phi=0$ in the cavity Λ the Hamiltonian of our model has the following conventional form (see Klemm and

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Zagrebnov 1977 and also Kittel 1963):

$$H_N = \omega_Q b_Q^\dagger b_Q + \epsilon \sum_{j=1}^{N} \sigma_j^z + \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \hat{\lambda}_j (\sigma_j^+ b_Q + \sigma_j^- b_Q^\dagger) + \Omega_Q a_Q^\dagger a_Q \tag{2.1}$$

where

$$\hat{\lambda}_j = \lambda \sin(Ql_j + Q\hat{u}_j), \qquad \hat{u}_j = \frac{a_Q^\dagger + a_Q}{\sqrt{(N\Omega_Q)}} \cos(Ql_j). \tag{2.2}$$

Here $l_j = aj$ and the Hilbert space of states $\mathscr{H} = \mathscr{H}_a \otimes \mathscr{H}_b \otimes \mathscr{H}_\sigma$ where $\mathscr{H}_a$ and $\mathscr{H}_b$ are respectively the Fock spaces of the creation–annihilation operators $(a_Q^\dagger, a_Q)$ (for phonons) and $(b_Q^\dagger, b_Q)$ (for photons); $\mathscr{H}_\sigma$ is the 2^N-dimensional space of states of the N two-level atoms with energy spacing ϵ, described by the spin-$\frac{1}{2}$ operators $\{\sigma_j^\alpha\}$: $\alpha = x, y, z$; $\sigma_j^\pm = \sigma_j^x \pm i\sigma_j^y$.

Proposition 2.1. Let operator H_N be defined by (2.1) and (2.2). Then H_N is self-adjoint on domain $D(T_N) = D(H_N)$, here $T_N = H_N(\lambda = 0)$ and $\exp(-H_N/\theta)$ is a trace-class operator for $\theta > 0$.

Proof. This may be performed in the manner of Hepp and Lieb (1973) or Zagrebnov *et al* (1975) if one notes that $\hat{\lambda}_j = \lambda \sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}]$ is a bounded operator on $\mathscr{H}_a$; therefore $N^{-1/2} \Sigma_{j=1}^N \hat{\lambda}_j(\sigma_j^+ b_Q + \sigma_j^- b_Q^\dagger)$ is a Kato perturbation of T_N (see, e.g. Kato 1966, Reed and Simon 1975).

Now, let $\mathscr{P}_n = P_a^{(n)} \otimes \mathbb{1}_b \otimes \mathbb{1}_\sigma$ be the projector onto the finite-dimensional subspace of the phonon states with less than or equal to n phonons so that $\mathscr{P}_n \to \mathbb{1}_a \otimes \mathbb{1}_b \otimes \mathbb{1}_\sigma$ strongly when $n \to \infty$. We define $H_N^{(n)} = \mathscr{P}_n H_N \mathscr{P}_n$ and consider the corresponding phonon finite-dimensional trace:

$$Z_n(\theta, N) = \mathrm{Tr}_{\mathscr{H}_a} \mathrm{Tr}_{\mathscr{H}_b} \mathrm{Tr}_{\mathscr{H}_\sigma} \mathscr{P}_n \exp(-H_N^{(n)}/\theta) = \mathrm{Tr}\, \mathscr{P}_n \exp(-H_N^{(n)}/\theta). \tag{2.3}$$

Proposition 2.2. Let $Z(\theta, N) = \mathrm{Tr} \exp(-H_N/\theta)$ be the partition function for our model (2.1), where θ is the temperature of the system. Then

$$\lim_{n\to\infty} Z_n(\theta, N) = Z(\theta, N). \tag{2.4}$$

Proof. The constructed sequence $\{\mathscr{P}_n\}$ forms the ascending discrete flag of projectors with $\mathscr{P}_n(\mathscr{H}_a \otimes D_b(H_N) \otimes \mathscr{H}_\sigma) \subset D(H_N)$ and $\bigcup_{n=1}^\infty \mathscr{P}_n(\mathscr{H}_a \otimes D_b(H_N) \otimes \mathscr{H}_\sigma) = \text{core } H_N$. Therefore the operators $\{\exp(-H_N^{(n)}/\theta)\}$ converge to $\exp(-H_N/\theta)$ in the trace-norm topology (Breitenecker 1973). But $\mathrm{Tr}(\cdot)$ is known to be continuous in the trace-norm topology (see, e.g. Kato 1966, Reed and Simon 1975), and this gives the desired result (2.4).

3. The free energy per particle

We start with the lower and upper bounds for the partition function of our model (2.4) using the cut-off coherent Glauber states for the phonons (for review see, e.g. Klauder and Sudarshan 1968 and the appendix):

$$|\alpha, n\rangle = P_a^{(n)} |\alpha\rangle. \tag{3.1}$$

Our approach follows in spirit the work of Hepp and Lieb (1973) generalising it to the coherent states both for photons and phonons.

3.1. Lower bound

Due to Hepp and Lieb (1973) we have for our model

$$Z_{-}(\theta, N) \leq Z(\theta, N) \tag{3.2}$$

where

$$Z_{-}(\theta, N) = \mathrm{Tr}_{\mathcal{H}_a} \frac{1}{\pi} \int_{\mathbb{C}^1} \mathrm{d}^2\beta \, \mathrm{Tr}_{\mathcal{H}_\sigma} \exp(-H_N(\beta, \beta^*)/\theta), \qquad \mathrm{d}^2\beta = \mathrm{d}(\mathrm{Re}\,\beta)\,\mathrm{d}(\mathrm{Im}\,\beta),$$

$$H_N(\beta, \beta^*) = \omega_Q |\beta|^2 + \epsilon \sum_{j=1}^{N} \sigma_j^z + \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} \sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}] \tag{3.3}$$
$$\times (\sigma_j^+ \beta + \sigma_j^- \beta^*) + \Omega_Q a_Q^\dagger a_Q.$$

Proposition 3.1. Let $Z_{-}(\theta, N)$ be the auxiliary function defined by (3.3), then

$$Z_0(\theta, N) \leq Z_{-}(\theta, N) \tag{3.4}$$

where

$$Z_0(\theta, N) = \frac{1}{\pi} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha \frac{1}{\pi} \int_{\mathbb{C}^1} \mathrm{d}^2\beta \, \mathrm{Tr}_{\mathcal{H}_\sigma} \exp(-H_N(\alpha, \alpha^*; \beta, \beta^*)/\theta),$$

$$H_N(\alpha, \alpha^*; \beta, \beta^*) = \omega_Q |\beta|^2 + \epsilon \sum_{j=1}^{N} \sigma_j^z + \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} \sin[(\alpha^* + \alpha)Q/\sqrt{(N\Omega_Q)}] \tag{3.5}$$
$$\times (\sigma_j^+ \beta + \sigma_j^- \beta^*) \exp(-Q^2/2N\Omega_Q) + \Omega_Q |\alpha|^2.$$

Proof. Use the phonon cut-off coherent state representation (3.1) for

$$Z_{-}^{(n)}(\theta, N) = \mathrm{Tr}_{\mathcal{H}_a} P_a^{(n)} \frac{1}{\pi} \int_{\mathbb{C}^1} \mathrm{d}^2\beta \mathrm{Tr}_{\mathcal{H}_\sigma} \exp(-H_N^{(n)}(\beta, \beta^*)/\theta)$$
$$= \frac{1}{\pi^2} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha \int_{\mathbb{C}^1} \mathrm{d}^2\beta \langle \alpha, n | \mathrm{Tr}_{\mathcal{H}_\sigma} \exp(-H_N^{(n)}(\beta, \beta^*)/\theta) | \alpha, n \rangle \tag{3.6}$$

with $H_N^{(n)}(\beta, \beta^*) = \mathcal{P}_n H_N(\beta, \beta^*) \mathcal{P}_n$, and the Peierls–Bogoliubov inequality $\langle \alpha, n | \exp(-H_N^{(n)}/\theta) | \alpha, n \rangle \geq \langle \alpha, n | \alpha, n \rangle \exp(-\langle \alpha, n | H_N^{(n)} | \alpha, n \rangle / \theta \langle \alpha, n | \alpha, n \rangle)$.

Then

$$Z_{-}^{(n)}(\theta, N) \geq \mathrm{Tr}_{\mathcal{H}_\sigma} \frac{1}{\pi^2} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha \int_{\mathbb{C}^1} \mathrm{d}^2\beta K_n(\alpha) \exp\Big[-\Big(\omega_Q |\beta|^2 + \epsilon \sum_{j=1}^{N} \sigma_j^z$$
$$+ \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} (\sigma_j^+ \beta + \sigma_j^- \beta^*) \langle \alpha, n | \sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}] | \alpha, n \rangle K_n^{-1}(\alpha)$$
$$+ \Omega_Q |\alpha|^2 \frac{K_{n-1}(\alpha)}{K_n(\alpha)} \Big) \theta^{-1} \Big]$$

where

$$K_n(\alpha) = \langle \alpha, n | \alpha, n \rangle = \exp(-|\alpha|^2) \sum_{l=0}^{n} |\alpha|^{2l}/l!.$$

The operator $\sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}]$ is bounded on $\mathscr{H}_a$. Thus from the strong convergence strong-$\lim_{n\to\infty} P_a^{(n)} = \mathbb{1}_a$ one has

$$\lim_{n\to\infty} \langle \alpha, n|\sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}]|\alpha, n\rangle = \langle \alpha|\sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}]|\alpha\rangle. \tag{3.7}$$

Now the right-hand side of (3.7) can be calculated by the Baker–Hausdorff formula. This, together with the dominated convergence theorem for $n\to\infty$ (see the appendix), proposition 2.2 and $\lim_{n\to\infty} K_n(\alpha) = 1$ prove the lower bound (3.4).

3.2. Upper bound

Also due to Hepp and Lieb (1973) one has, for the partition function of our model,

$$Z(\theta, N) \leq Z_-(\theta, N)\exp(\omega_Q/\theta). \tag{3.8}$$

Proposition 3.2. Let $Z_-(\theta, N)$ be the auxiliary function defined by (3.3), then

$$Z_-(\theta, N) \leq Z_0(\theta, N)\exp(\Omega_Q/\theta). \tag{3.9}$$

Proof. According to Lieb (1973) we define (see § 2 and (3.3))

$$\begin{gathered} Z_m^{(n)} = \frac{1}{\pi}\int_{\mathbb{C}^1} \mathrm{d}^2\beta[\exp(-\omega_Q|\beta|^2/\theta)]\,\mathrm{Tr}_{\mathscr{H}_a} P_a^{(n)}\,\mathrm{Tr}_{\mathscr{H}_\sigma}(1 - \tilde{H}_N^{(n)}(\beta, \beta^*)/m\theta)^m \\ \tilde{H}_N^{(n)}(\beta, \beta^*) = \mathscr{P}_n H_N(\beta, \beta^*)\mathscr{P}_n - \omega_Q|\beta|^2. \end{gathered} \tag{3.10}$$

Since the trace in (3.10) is finite dimensional, $\lim_{m\to\infty} Z_m^{(n)} = Z_-^{(n)}$ (see (3.6)). Now it is convenient to substitute Hamiltonian $\tilde{H}_N(\beta, \beta^*)$ in (3.10) by its 'diagonal' phonon-coherent state representation $\hat{H}_N(\alpha, \beta, \epsilon)$ (see the appendix) with a convergence factor, which preserves the rigour of our construction. Here we use the following formulae (see (A.2) and (A.3)):

$$\begin{aligned} \{a_Q^\dagger a_Q\}_{\epsilon>0} &= \frac{1}{\pi}\int_{\mathbb{C}^1} \mathrm{d}^2\alpha(|\alpha|^2 - 1)[\exp(-\epsilon|\alpha|^2)]|\alpha\rangle\langle\alpha|, \\ \{\sin[(a_Q^\dagger + a_Q)Q/\sqrt{(N\Omega_Q)}]\}_{\epsilon>0} &\\ &= \frac{1}{\pi}\int_{\mathbb{C}^1} \mathrm{d}^2\alpha\{\sin[(\alpha^* + \alpha)Q/\sqrt{(N\Omega_Q)}]\}[\exp(-Q^2/2N\Omega_Q)] \\ &\quad\times[\exp(-\epsilon|\alpha|^2)]|\alpha\rangle\langle\alpha|. \end{aligned} \tag{3.11}$$

Therefore

$$\begin{gathered} \tilde{H}_N(\beta, \beta^*) \to \hat{\tilde{H}}_N(\alpha, \beta, \epsilon) = \hat{H}_N(\alpha, \beta, \epsilon) - \omega_Q|\beta|^2, \\ \lim_{\epsilon\to+0} Z_-^{(n)}(\hat{H}_N(\alpha, \beta, \epsilon)) = Z_-^{(n)}, \qquad \lim_{m\to\infty} Z_m^{(n)}(\hat{\tilde{H}}_N(\alpha, \beta, \epsilon)) = Z_-^{(n)}(\epsilon). \end{gathered}$$

For $Z_m^{(n)}(\hat{\tilde{H}}_N(\alpha, \beta, \epsilon)) = Z_m^{(n)}(\epsilon)$ as shown by Lieb (1973), one has

$$\begin{aligned} Z_m^{(n)}(\epsilon) &\leq \frac{1}{\pi^2}\int_{\mathbb{C}^1} \mathrm{d}^2\alpha K_n(\alpha)\int_{\mathbb{C}^1} \mathrm{d}^2\beta[\exp(-\omega_Q|\beta|^2/\theta)]\mathrm{Tr}_{\mathscr{H}_\sigma}(1 - \tilde{H}_N(\alpha, \beta, \epsilon)/m\theta)^m, \\ \tilde{H}_N(\alpha, \beta, \epsilon) &= \epsilon\sum_{j=1}^N \sigma_j^z + \frac{\lambda}{\sqrt{N}}\sum_{j=1}^N \{\sin[(\alpha^* + \alpha)Q/\sqrt{(N\Omega_Q)}]\}[\exp(-Q^2/2N\Omega_Q)] \\ &\quad\times[\exp(-\epsilon|\alpha|^2)](\sigma_j^+\beta + \sigma_j^-\beta^*) + \Omega_Q(|\alpha|^2 - 1)\exp(-\epsilon|\alpha|^2). \end{aligned} \tag{3.12}$$

The convergence factor $\exp(-\epsilon|\alpha|^2)$ and Gaussian decrease of $K_n(\alpha)$ allow us to use the dominated convergence theorem to assert that

$$Z_-^{(n)}(\epsilon) \leq \frac{1}{\pi^2} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha K_n(\alpha) \int_{\mathbb{C}^1} \mathrm{d}^2\beta \, \mathrm{Tr}_{\mathscr{H}_\sigma}[\exp(-\tilde{H}_N(\alpha, \beta, \epsilon)/\theta)][\exp(-\omega_Q|\beta|^2/\theta)]$$

and further to let $\epsilon \to +0$ (see (3.12)):

$$Z_-^{(n)} \leq \frac{1}{\pi^2} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha K_n(\alpha) \int_{\mathbb{C}^1} \mathrm{d}^2\beta \, \mathrm{Tr}_{\mathscr{H}_\sigma}[\exp(-H_N(\alpha, \alpha^*; \beta, \beta^*)/\theta)] \exp(\Omega_Q/\theta). \quad (3.13)$$

Hamiltonian $H_N(\alpha, \alpha^*; \beta, \beta^*)$ has a term $\Omega_Q|\alpha|^2$ (see (3.5)) so one can use the dominated convergence theorem for $n \to \infty$ and proposition 2.2 to obtain (3.9).

Now we need the following proposition.

Proposition 3.3. Let $Z_0(\theta, N) \equiv Z_0(\theta, N|\lambda_N = \lambda \exp(-Q^2/2N\Omega_Q))$ be the partition function defined by (3.5). Then for the corresponding free energy per atom $f_N^{(0)}(\theta, \lambda_N) = -(\theta/N) \ln Z_0(\theta, N|\lambda_N)$

$$\lim_{N\to\infty} f_N^{(0)}(\theta, \lambda_N) = f_0(\theta, \lambda) \quad (3.14)$$

where

$$f_0(\theta, \lambda) = \lim_{N\to\infty} f_N^{(0)}(\theta, \lambda). \quad (3.15)$$

Proof. From the Bogoliubov inequality (convexity of the $f_N(\theta, \xi)$ with respect to $\xi \in \mathbb{R}^1$) one has

$$\Delta_N \frac{1}{N}\langle H_I\rangle_{\xi=\lambda_N} \leq f_N^{(0)}(\theta, \lambda_N) - f_N^{(0)}(\theta, \lambda) \leq \Delta_N \frac{1}{N}\langle H_I\rangle_{\xi=\lambda}, \quad (3.16)$$

$$\Delta_N H_I = H_N(\alpha, \alpha^*; \beta, \beta^*|\lambda_N) - H_N(\alpha, \alpha^*; \beta, \beta^*|\lambda), \qquad \Delta_N = [\exp(-Q^2/2N\Omega_Q)] - 1;$$

$$H_I = \frac{\lambda}{\sqrt{N}} \sum_{j=1}^{N} \{\sin[(\alpha^* + \alpha)Q/\sqrt{(N\Omega_Q)}]\}(\sigma_j^+\beta + \sigma_j^-\beta^*) \quad (3.17)$$

and (see (3.5))

$$\langle H_I\rangle_\xi = Z_0^{-1}(\theta, N|\xi) \frac{1}{\pi^2} \int_{\mathbb{C}^1} \mathrm{d}^2\alpha \int_{\mathbb{C}^1} \mathrm{d}^2\beta \mathrm{Tr}_{\mathscr{H}_\sigma}\{H_I \exp[-H_N(\alpha, \alpha^*; \beta, \beta^*|\xi)/\theta]\}.$$

But $|(1/N)\langle H_I\rangle_\xi|$ is clearly bounded by a continuous function $c(\theta, \xi)$, therefore (3.14) is an immediate consequence of (3.15)–(3.17).

Corollary 3.1. Comparing (3.2), (3.4) and (3.8), (3.9), one has from (3.14), (3.15)

$$\lim_{N\to\infty} \left(-\frac{\theta}{N} \ln Z(\theta, N)\right) = f_0(\theta, \lambda). \quad (3.18)$$

4. Conclusion

For the free energy per particle $f_N(\theta) = -(\theta/N) \ln Z(\theta, N)$ of our model (2.1) for the matter interacting with radiation we obtain:

(i) the thermodynamic limit $\lim_{N\to\infty} f_N(\theta)$ exists and coincides with $f_0(\theta, \lambda)$ (see (3.18));
(ii) $f_0(\theta, \lambda)$ can be evaluated exactly from (3.5) by the steepest descent method and it is evidently equal to that for the classical vibrations (Zagrebnov and Klemm 1976, Klemm and Zagrebnov 1977).

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Appendix

First we remind the reader of the dominated convergence theorem (see, e.g. Kato 1966, Reed and Simon 1975).

Theorem (Lebesgue). Let $\{F_n(x)\}$ be a sequence of real functions with $x \in \mathbb{R}^1$ such that $F_n(x) \in L^1(\mathbb{R}^1)$ and $\lim_{n\to\infty} F_n(x) = F(x)$ almost everywhere. If there is a $G(x) \in L^1(\mathbb{R}^1)$ with $|F_n(x)| \leq G(x)$ almost everywhere, then
(i) $F(x) \in L^1(\mathbb{R}^1)$;
(ii) $\lim_{n\to\infty} \|F - F_n\|_{L^1(\mathbb{R}^1)} = 0$.

Secondly, let $\mathcal{H}_a$ be the Fock space for a given boson mode $(a^\dagger, a)$ with the vacuum $|0\rangle_a$. Then for any complex number $z \in \mathbb{C}^1$ a Glauber coherent state is

$$|z\rangle = [\exp(-|z|^2/2)] \sum_{n=0}^{\infty} z^n \frac{(a^\dagger)^n}{n!} |0\rangle_a. \tag{A.1}$$

For $z \in \mathbb{C}^1$ the coherent states $\{|z\rangle\}$ form an overcomplete set of the vectors in $\mathcal{H}_a$. The important peculiarity of this property is expressed by the following theorem.

Theorem (Mehta and Sudarshan 1965, Klauder *et al* 1965). Let A be an operator with a dense domain $D(A) \subset \mathcal{H}_a$ and $|n\rangle \in D(A)$ for any n, here $|n\rangle = [(a^\dagger)^n/\sqrt{n!}]|0\rangle_a$. If the series $\sum_{n,m=0}^{\infty} [\langle n|A|m\rangle/\sqrt{(n!m!)}](z_1^*)^n (z_2)^m$ is absolutely convergent for all finite values of $|z_1|$, $|z_2|$, then
(i) the operator A is uniquely defined by its diagonal elements $\langle z|A|z\rangle$, $z \in \mathbb{C}^1$;
(ii) for the A one has a 'diagonal' coherent-state representation:

$$A = \frac{1}{\pi} \int_{\mathbb{C}^1} d^2z\, \phi(z) |z\rangle\langle z|, \qquad d^2z = d(\operatorname{Re} z)\, d(\operatorname{Im} z), \tag{A.2}$$

where $\phi(z)$ is in general a distribution defined by the following equation:

$$\langle z|A|z\rangle = \frac{1}{\pi} \int_{\mathbb{C}^1} d^2z' \phi(z') \exp(-|z - z'|^2). \tag{A.3}$$

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