Thermodynamic properties of cavity-assisted many-body atomic systems

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We consider an ensemble of N two-level atoms coupled by two photon Raman transition, and atoms are placed in a cavity. Atoms and photons are expected to interact in a highly nonlinear fashion, though atom themselves are considered non-interacting. We don't consider cavity pump and decay in this work.

Using bare atomic psedo-spin operater $\Psi_\sigma(\mathbf{r})$ and photon field operater c (without explicit time dependence), we can write the atom-cavity Hamiltonian as,

$$H = \sum_{j=1}^{N}\sum_{\sigma}\int d\mathbf{r}\left[\Psi^\dagger_{j\sigma}(\mathbf{r})\left(\frac{\hbar^2\hat{\mathbf{k}}^2}{2m}+\epsilon^0_\sigma\right)\Psi_{j\sigma}(\mathbf{r})\right]+\frac{\Omega}{2}\sum_{j=1}^{N}\int d\mathbf{r}\left(e^{2i\hbar k_r z}\Psi^\dagger_{j\uparrow}(\mathbf{r})\Psi_{j\downarrow}(\mathbf{r})ce^{-i\omega_R t}+c.c\right)+\hbar\omega_c c^\dagger c$$

We work in rotating frame $\tilde{c} = ce^{-i\omega_R t}$ and gauge transformation $\tilde{\psi}_{j\uparrow} = \Psi_{j\uparrow}e^{-i\hbar k_r z}$, $\tilde{\psi}_{j\downarrow} = \Psi_{j\downarrow}e^{+i\hbar k_r z}$. After unitary transformation of origional Hamiltonian, we can write

$$H = \sum_{j=1}^{N}\int d\mathbf{r}\left[\begin{pmatrix}\tilde{\psi}^\dagger_{j\uparrow}(\mathbf{r}) & \tilde{\psi}^\dagger_{j\downarrow}(\mathbf{r})\end{pmatrix}\left[\frac{\hbar^2\hat{\mathbf{k}}^2}{2m}+\frac{\hbar^2}{m}k_r\hat{k}_z\sigma_{jz}+\delta\sigma_{jz}\right]\begin{pmatrix}\tilde{\psi}_{j\uparrow}(\mathbf{r})\\ \tilde{\psi}_{j\downarrow}(\mathbf{r})\end{pmatrix}+\frac{\Omega}{2}\tilde{\psi}^\dagger_{j\uparrow}(\mathbf{r})\tilde{\psi}_{j\downarrow}(\mathbf{r})\tilde{c}+c.c\right]+\omega_c\tilde{c}^\dagger\tilde{c} \quad (1)$$

where we have neglected constant energy $\frac{\hbar^2 k_r^2}{2m}$ and incorprated energy shift of two-photon detunning into δ. From now on, we drop tilde symbol. Writing the operator in momentum space, we write $\tilde{\psi}_{j\sigma}(\mathbf{r}) = \frac{V}{(2\pi)^3}\int d\mathbf{k}e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\psi}_{j\sigma}(\mathbf{k})$ and Eq. 1 is reduced to,

$$H = \omega_c\tilde{c}^\dagger\tilde{c}+\sum_{j=1}^{N}\sum_{\mathbf{k}}\left[\left(h_1(\mathbf{k})\hat{\psi}^\dagger_{j\uparrow}(\mathbf{k})\hat{\psi}_{j\uparrow}(\mathbf{k})+h_2(\mathbf{k})\hat{\psi}^\dagger_{j\downarrow}(\mathbf{k})\hat{\psi}_{j\downarrow}(\mathbf{k})\right)+\frac{\Omega}{2}\left(\hat{\psi}^\dagger_{j\uparrow}(\mathbf{k})\hat{\psi}_{j\downarrow}(\mathbf{k})\tilde{c}+\tilde{c}^\dagger\hat{\psi}^\dagger_{j\downarrow}(\mathbf{k})\hat{\psi}_{j\uparrow}(\mathbf{k})\right)\right] \quad (2)$$

where $h_1(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m}+\frac{\hbar^2}{m}k_r k_z+\delta$ and $h_2(\mathbf{k}) = \frac{\hbar^2\mathbf{k}^2}{2m}-\frac{\hbar^2}{m}k_r k_z-\delta$. The thermodynamic functions can be calculated from the canonical partition function, $Z(N,T) = \mathrm{Tr}[e^{-\beta H}]$. A convenient basis to calculate the trace of the partition function is the Glauber's coherent state $|\alpha\rangle$ for the photon field, then we have

$$Z(N,T) = \sum_{s_1=\uparrow,\downarrow}\ldots\sum_{s_N=\uparrow,\downarrow}\frac{V}{(2\pi)^3}\int d\mathbf{k}_1\ldots\frac{V}{(2\pi)^3}\int d\mathbf{k}_N\int\frac{d^2\alpha}{\pi}\langle\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N|\langle\alpha|e^{-\beta H}|\alpha\rangle|\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N\rangle \quad (3)$$

where atomic field is denoted by atom index j and momentum $\mathbf{k}$ and spin $\sigma=\uparrow,\downarrow$. It follows then that the expectation value becomes,

$$\langle\alpha|e^{-\beta H}|\alpha\rangle = \exp\left\{-\beta\omega_c|\alpha|^2-\beta\sum_{j=1}^{N}\sum_{\mathbf{k}}h_j(\mathbf{k})\right\} \quad (4)$$

$$h_j(\mathbf{k}) = \left(h_1(\mathbf{k})\hat{\psi}^\dagger_{j\uparrow}(\mathbf{k})\hat{\psi}_{j\uparrow}(\mathbf{k})+h_2(\mathbf{k})\hat{\psi}^\dagger_{j\downarrow}(\mathbf{k})\hat{\psi}_{j\downarrow}(\mathbf{k})\right)+\frac{\Omega}{2}\left(\hat{\psi}^\dagger_{j\uparrow}(\mathbf{k})\hat{\psi}_{j\downarrow}(\mathbf{k})\alpha+\hat{\psi}^\dagger_{j\downarrow}(\mathbf{k})\hat{\psi}_{j\uparrow}(\mathbf{k})\alpha^*\right) \quad (5)$$

and using the property $[h_i(\mathbf{k}), h_j(\mathbf{k}')] = 0$, we can reduce integrand of Eq. 3 to

$$\begin{aligned}
\langle\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N|\langle\alpha|e^{-\beta H}|\alpha\rangle|\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N\rangle &= e^{-\beta\omega_c|\alpha|^2}\langle\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N|e^{-\beta\sum_{j=1}^{N}\sum_{\mathbf{k}}h_j(\mathbf{k})}|\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N\rangle && (6)\\
&= e^{-\beta\omega_c|\alpha|^2}\langle\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N|\prod_{j=1}^{N}\prod_{\mathbf{k}=-\infty}^{\infty}e^{-\beta h_j(\mathbf{k})}|\mathbf{k}_1 s_1;\ldots;\mathbf{k}_N s_N\rangle && (7)\\
&= e^{-\beta\omega_c|\alpha|^2}\prod_{j=1}^{N}\langle\mathbf{k}_j s_j|e^{-\beta h_j(\mathbf{k}_j)}|\mathbf{k}_j s_j\rangle && (8)
\end{aligned}$$

From Eq. 3 and Eq. 8, we have

$$
\begin{aligned}
Z(N,T) &= \sum_{s_1=\uparrow,\downarrow} ... \sum_{s_N=\uparrow,\downarrow} \frac{V}{(2\pi)^3}\int d\mathbf{k}_1 ... \frac{V}{(2\pi)^3}\int d\mathbf{k}_N \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left(\prod_{j=1}^{N} \langle \mathbf{k}_j s_j | e^{-\beta h_j(\mathbf{k}_j)} | \mathbf{k}_j s_j\rangle\right) && (9)\\
&= \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left\{ \frac{V}{(2\pi)^3}\int d\mathbf{k}_j \mathrm{Tr}_\sigma \exp\left[-\beta \begin{pmatrix} h_1(\mathbf{k}_j) & \frac{\Omega}{2}\alpha \\ \frac{\Omega}{2}\alpha^* & h_2(\mathbf{k}_j) \end{pmatrix}\right]\right\}^N && (10)
\end{aligned}
$$

where the Trace is only for spin degrees of freedom. The eigenvalue of the 2×2 matrix is given by

$$
\epsilon_j^{\pm}(\mathbf{k}_j) = \frac{\hbar^2\mathbf{k}_j^2}{2m} \pm \sqrt{\left(\frac{\hbar^2}{m}k_r k_{jz} + \delta\right)^2 + \left(\frac{\Omega}{2}\right)^2 |\alpha|^2} \equiv \frac{\hbar^2\mathbf{k}_j^2}{2m} \pm |\mu(\mathbf{k}_j)| \tag{11}
$$

Then from Eq. 10 we have,

$$
\begin{aligned}
Z(N,T) &= \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left[\frac{V}{(2\pi)^3}\int d\mathbf{k}_j \left(e^{-\beta\epsilon_j^+(\mathbf{k}_j)} + e^{-\beta\epsilon_j^-(\mathbf{k}_j)}\right)\right]^N && (12)\\
&= \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left[\frac{V}{(2\pi)^3}\int d\mathbf{k} \exp(-\beta\frac{\hbar^2\mathbf{k}^2}{2m}) \left(e^{-\beta|\mu(\mathbf{k})|} + e^{\beta|\mu(\mathbf{k})|}\right)\right]^N && (13)\\
&= \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left[\frac{V}{(2\pi)^3}\int d\mathbf{k} \exp(-\beta\frac{\hbar^2\mathbf{k}^2}{2m}) 2\cosh\beta\sqrt{\left(\frac{\hbar^2}{m}k_r k_z + \delta\right)^2 + \left(\frac{\Omega}{2}\right)^2 |\alpha|^2}\right]^N && (14)\\
&= \left[\frac{V}{(2\pi)^3}\int dk_x \int dk_y \exp(-\beta\frac{\hbar^2(k_x^2+k_y^2)}{2m})\right]^N && (15)\\
&\times \int \frac{d^2\alpha}{\pi} e^{-\beta\omega_c|\alpha|^2} \left(\int dk_z \exp(-\beta\frac{\hbar^2k_z^2}{2m}) 2\cosh(\beta\sqrt{\left(\frac{\hbar^2}{m}k_r k_z + \delta\right)^2 + \left(\frac{\Omega}{2}\right)^2 |\alpha|^2})\right)^N && (16)\\
&= \left(\frac{V}{(2\pi)^3}\frac{2\pi m}{\hbar^2\beta}\right)^N 2\int_0^\infty r e^{-\beta\omega_c r^2} dr \left(\int dk_z \exp(-\beta\frac{\hbar^2k_z^2}{2m}) 2\cosh(\beta\sqrt{\left(\frac{\hbar^2}{m}k_r k_z + \delta\right)^2 + \left(\frac{\Omega}{2}\right)^2 r^2})\right)^N && (17)
\end{aligned}
$$

In canonical ensemble and thermodynamic limit, free energy per particle is given by

$$
f(T,\Omega,\omega_c,\delta) = -\frac{1}{\beta}\lim_{N\to\infty}\frac{\log Z(N,T)}{N} \tag{18}
$$

and we need to seek phase transition property by studying saddle point solution to F energy landscapes.

Although we could take the limit of $N\to\infty$ numerically, we shall make use of Laplace's method to further reduce the integrals. The formal statement of Lapace's method is:

Assume that $f(x)$ is a twice differentiable function on $[a,b]$ with $x_0 \in [a,b]$ the unique point such that $f(x_0) = \max_{[a,b]} f(x)$. Assume additionally that $f''(x_0) < 0$, then

$$
\lim_{N\to+\infty}\left(\frac{\int_a^b e^{Nf(x)}dx}{e^{Nf(x_0)}\sqrt{\frac{2\pi}{-Nf''(x_0)}}}\right) = 1 \tag{19}
$$

We denote,

$$
\mathcal{S} = \int dk_z \exp(-\beta\frac{\hbar^2k_z^2}{2m}) 2\cosh(\beta\sqrt{\left(\frac{\hbar^2}{m}k_r k_z + \delta\right)^2 + \left(\frac{\sqrt{N}\Omega}{2}\right)^2 \frac{|\alpha|^2}{N}}) \tag{20}
$$

Then, partition function is formally written as

$$
\begin{aligned}
Z(N,T) &= \left(\frac{V}{(2\pi)^3}\frac{2\pi m}{\hbar^2\beta}\right)^N 2\int_0^\infty r e^{-N\frac{\beta\omega_c r^2}{N}} e^{N\log\mathcal{S}} dr && (21)\\
&= N\left(\frac{V}{(2\pi)^3}\frac{2\pi m}{\hbar^2\beta}\right)^N \int_0^\infty dy \exp\left\{N\left[-\beta\omega_c y + \log\mathcal{S}\right]\right\} && (22)
\end{aligned}
$$

where we have denoted $y = \frac{|\alpha|^2}{N}$. By Laplace's method, the integral is given by

$$Z(N,T) = N\frac{1}{\sqrt{N}}\sqrt{\frac{2\pi}{-\phi''(y_0)}}\left(\frac{V}{(2\pi)^3}\frac{2\pi m}{\hbar^2\beta}\right)^N \max_{0\le y\le\infty} \exp\{N\phi(y)\} \tag{23}$$

where y_0 is the point that gives maximum and $\phi(y) = -\beta\omega_c y + \log\mathcal{S}$. Then

$$\phi'(y) = -\beta\omega_c + \frac{\beta\int dk_z \exp(-\beta\frac{\hbar^2k_z^2}{2m})\sinh\left(\beta\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}\right)\frac{\left(\frac{\sqrt{N}\Omega}{2}\right)^2}{\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}}}{\mathcal{S}} \tag{24}$$

Putting $\phi'(y) = 0$ we get an integral equation of $\eta = \sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}$, and we shall denote $\tilde{\Omega} = \sqrt{N}\Omega$ is the Tavis-Cummings coupling constant, an enhancement of coupling strength which scales as $\sqrt{N}$.

$$\omega_c\int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})2\cosh(\beta\eta) = \int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})\sinh(\beta\eta)\frac{\left(\frac{\sqrt{N}\Omega}{2}\right)^2}{\eta} \tag{25}$$

where k_z is yet to be integrated out. Then,

$$-\beta f(T,\Omega,\omega_c,\delta) \propto \phi(y_0) \tag{26}$$

Second order derivative can be checked straightforwardly,

$$\phi''(y) = \frac{\frac{\partial Q}{\partial y}\mathcal{S} - Q^2}{\mathcal{S}^2} \tag{27}$$

where $Q \equiv \frac{\partial\mathcal{S}}{\partial y} = \beta\int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})\sinh\left(\beta\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}\right)\frac{\left(\frac{\sqrt{N}\Omega}{2}\right)^2}{\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}}$ and

$$\begin{aligned}
\frac{\partial Q}{\partial y} &= \beta\left(\frac{\sqrt{N}\Omega}{2}\right)^2\int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})\partial_y\left(\frac{\sinh\left(\beta\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}\right)}{\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}}\right) \\
&= \beta\left(\frac{\sqrt{N}\Omega}{2}\right)^4\int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})\frac{\frac{\beta}{2}\cosh\left(\beta\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}\right) - \frac{\sinh\left(\beta\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}\right)}{2\sqrt{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y}}}{\left(\frac{\hbar^2}{m}k_rk_z+\delta\right)^2+\left(\frac{\sqrt{N}\Omega}{2}\right)^2y} && (28) \\
&= \beta\left(\frac{\sqrt{N}\Omega}{2}\right)^4\int dk_z\exp(-\beta\frac{\hbar^2k_z^2}{2m})\frac{\frac{\beta}{2}\cosh(\beta\eta) - \frac{\sinh(\beta\eta)}{2\eta}}{\eta^2} && (29)
\end{aligned}$$

With the optimality condition computed, it is helpful to compute the average photon number,

$$\begin{aligned}
\langle\frac{a^\dagger a}{N}\rangle &= \frac{\mathrm{Tr}[a^\dagger ae^{-\beta H}/N]}{Z(N,T)} && (30) \\
&= \frac{|\alpha|^2}{N} && (31) \\
&= y_0 && (32)
\end{aligned}$$