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A theorem on the generic form of the quantum cluster integral

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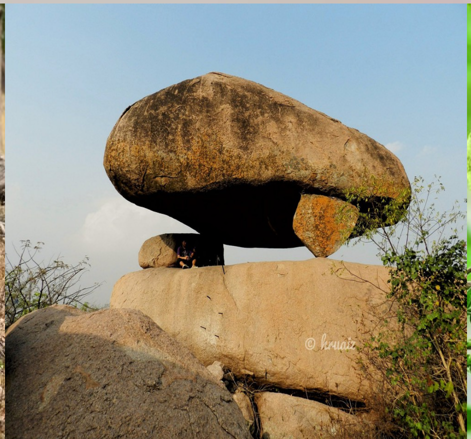


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Plan of my talk

1. Introduction of the cluster expansion for an interacting classical gas

2. Quantum cluster expansion for a free Bose or Fermi gas

3. Quantum cluster integral for a Bose or Fermi gas in any restricted geometry

4. Our theorem on the generic form of the cluster integral

5. Conclusions

Introduction: Cluster expansion for a classical gas

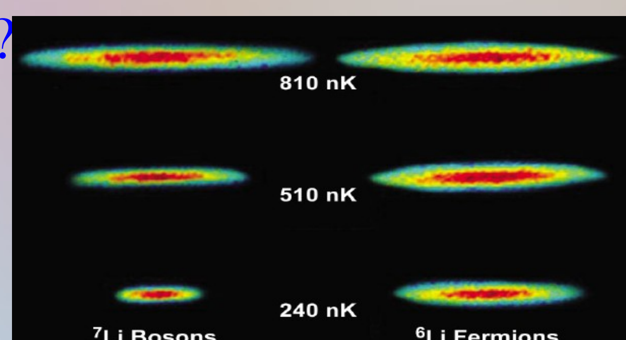
The Mayer (classical) cluster expansion of the grand free energy for an interacting classical gas takes the form

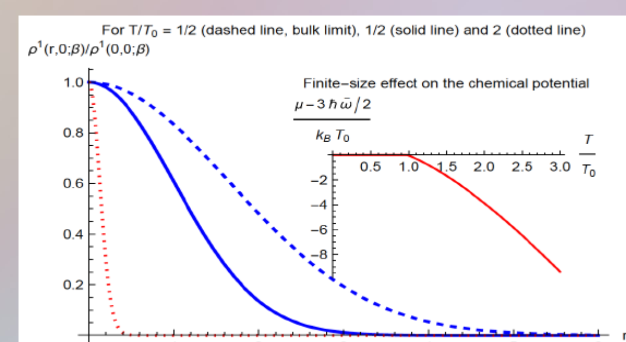
$$\Omega = -pV = -k_B T \sum_{\nu=1}^{\infty} \frac{h_\nu z^\nu}{\nu}$$

where z is the fugacity and h_ν is the ν-cluster integral for a cluster of ν particles in the gas (*Mayer et al, Statistical Mechanics, 1940*). For such a system we have the following results.

$$h_1 = \frac{V}{\lambda_T^3} \qquad h_2 = \frac{2}{2!\lambda_T^6}\int\int\left[-1+e^{-\frac{V_{int}(|\vec{r}_2-\vec{r}_1|)}{k_B T}}\right]d^3\vec{r}_1 d^3\vec{r}_2 \qquad \lambda_T = \sqrt{\frac{2\pi\hbar^2}{mk_BT}} \qquad z = e^{\mu/k_B T}$$

What would be the cluster expansion for a quantum gas in a harmonic trap which drew enormous interest in the last two and half decades in connection with the ultracold atoms?





Quantum cluster expansion and the quantum cluster integral

Though the cluster integrals ($\{h_\nu\}$) are different for different systems, the form of the classical cluster expansion does not change even for an ideal quantum (Bose or Fermi) gas. The generic form of the quantum cluster expansion of an ideal Bose or Fermi gas takes the form (*Kahn-Uhlenbeck, Physica, 1938*)

$$\Omega = -k_B T \sum_{\nu=1}^{\infty} \frac{h_\nu z^\nu}{\nu}$$

where the quantum cluster integrals takes the form (*Feynman, Stat. Mech., 1972*)

$$h_\nu = (\pm 1)^{\nu-1} \int ... \int \rho(\vec{r}_1, \vec{r}_2; \beta)\rho(\vec{r}_2, \vec{r}_3; \beta)...\rho(\vec{r}_\nu, \vec{r}_1; \beta)\mathrm{d}^3\vec{r}_1...\mathrm{d}^3\vec{r}_\nu$$

and $\rho(\vec{r}_i, \vec{r}_j; \beta) = \langle \vec{r}_i | \hat{\rho} | \vec{r}_j \rangle \ = \ \langle \vec{r}_i | \mathrm{e}^{-\beta \hat{H}} | \vec{r}_j \rangle$

is an element of the unnormalized density matrix for a single particle of the quantum gas. This form though was initially proposed for free Bose or Fermi gas, it remain unaltered even for any trapped ideal quantum gas. The ν-quantum cluster integral h_ν for the ideal quantum gas arises purely from the exchange effect with cyclic permutation within the cluster of ν particles in the system. The generic form of h_ν has not been obtained before us. Evaluation of the quantum cluster integral seems difficult because the individual density matrix elements in h_ν are not independent. We can, however, overcome the difficulty by applying our theorem where completeness of the position kets plays a significant role.

Our theorem with a proof

$$h_\nu = (\pm 1)^{\nu-1} \int .. \int \rho(\vec{r}_1, \vec{r}_2) ... \rho(\vec{r}_{\nu-1}, \vec{r}_\nu) \rho(\vec{r}_\nu, \vec{r}_1) \mathrm{d}^3\vec{r}_1 .. \mathrm{d}^3\vec{r}_\nu$$

$$= (\pm 1)^{\nu-1} [\prod_{j=1}^{\nu} \int \mathrm{d}^3\vec{r}_j] \langle \vec{r}_1|\hat{\rho}|\vec{r}_2\rangle .. \langle \vec{r}_{j-2}|\hat{\rho}|\vec{r}_{j-1}\rangle \langle \vec{r}_{j-1}|\hat{\rho}|\vec{r}_j\rangle ... \langle \vec{r}_\nu|\hat{\rho}|\vec{r}_1\rangle$$

$$= (\pm 1)^{\nu-1} \int \mathrm{d}\vec{r}_1 \langle \vec{r}_1|\hat{\rho}^\nu|r_1\rangle$$

$$\mathrm{Tr.}(\hat{\rho}^\nu) = \mathrm{Tr.}(\mathrm{e}^{-\nu\beta\hat{H}})$$

$$= (\pm 1)^{\nu-1} \sum_{j_1, j_2, j_3} \mathrm{e}^{-\beta\nu E_{j_1, j_2, j_3}}$$

where E_{j_1,j_2,j_3} is the energy eigenvalue in the single-particle sate $\psi_{j_1,j_2,j_3}(\vec{r})$ and the summation over j_1, j_2, j_3 are taken over the complete and orthonormal set of the single-particle states. Hence, we obtain the quantum cluster integral for the cycle of the length ν as

$$h_\nu = (\pm 1)^{\nu-1} \sum_{j_1, j_2, j_3} \mathrm{e}^{-\beta\nu E_{j_1, j_2, j_3}} = (\pm 1)^{\nu-1} Z(\nu\beta)$$

where $Z(\nu\beta)$ is the canonical partition function for a composite particle composed of the ν indistinguishable constituent particles in the cluster of size ν at a temperature $T = 1/k_B\beta$. It is to be noted that, the energy is an extensive variable at least for the ideal gas of particles. So, the energy of the composite particle in a given energy eigenstate $|\psi_{j_1,j_2,j_3}\rangle$ is ν times the energy of a constituent particle in the same eigenstate in the cluster of size ν.

The statement of the theorem and conclusions

• Our Theorem: The generic form of the quantum cluster integral for a cluster of size ν of any system of ideal indistinguishable bosons (upper sign) or fermions (lower sign) in thermodynamic equilibrium would be $(\pm 1)^{\nu}$ times the canonical partition function of a single composite particle composed of ν bosons or fermions in the cluster [S. Dey, P. Manchala1, S. Basu, D. Banerjee, and S. Biswas, Physica Scripta 95, 075003 (2020)].

•By applying the theorem, we have obtained quantum cluster expansion of the grand free energy in a closed form for an ideal Bose or Fermi gas in both the 3-D box geometry and the harmonically trapped geometry [S. Dey, P. Manchala1, S. Basu, D. Banerjee, and S. Biswas, Physica Scripta 95, 075003 (2020)].

•Our theorem for the quantum cluster integral is generic for ideal quantum (Bose or Fermi) gas. It could be any free gas or any trapped gas in thermodynamic equilibrium.

• No approximations are involved in our proof. Hence, our theorem can be useful to capture exact finite-size effect on any quantum (Bose or Fermi) gas.

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2. **SERB, DST, Govt. of India**
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3. 

Thanks to all of you for your kind attention.