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Rotating Isotropic Harmonic Oscillator

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Abstract

We study the properties of the isotropic harmonic oscillator under rotation, and further we extend the partition function to include the spin contributions in order to have a complete description of the system. Applying the statistical mechanics techniques, we study the system from both classical and quantum point of view. We point out that all observables diverge as the rotation parameter approaches the oscillator strength, i.e. $\Omega \to \omega$.

1 Thermodynamics and statistical mechanics

- We consider the 3D harmonic oscillator under rotation, described by the density operator

$$\rho = e^{-\beta(H-\mathbf{\Omega}\cdot\mathbf{L}-\mathbf{\Omega}_\Sigma\cdot\mathbf{\Sigma})}, \qquad H = \frac{\boldsymbol{P}}{2m} + \frac{1}{2}m\omega^2\boldsymbol{r}^2,$$

with $H \equiv$ Hamiltonian, $\mathbf{L} \equiv$ orbital angular momentum, $\mathbf{\Sigma} \equiv$ spin angular momentum, $\beta = 1/k_BT \equiv$ inverse temperature, $\mathbf{\Omega} \equiv$ angular velocity, $\mathbf{\Omega}_\Sigma \equiv$ spin potential.

- Denoting $Z = \mathrm{Tr}(\rho) \equiv$ partition function and $F = -k_BT\ln Z$ the free energy, the entropy S, $\mathbf{L}$ and $\mathbf{\Sigma}$ are given by [1]

$$S = -\frac{\partial F}{\partial T}, \qquad \mathbf{L} = -\frac{\partial F}{\partial \mathbf{\Omega}}, \qquad \mathbf{\Sigma} = -\frac{\partial F}{\partial \mathbf{\Omega}_\Sigma}.$$

Thermodynamic consistency is ensured by the Euler relation: $E = ST + F + \mathbf{\Omega}\cdot\mathbf{L} + \mathbf{\Omega}_\Sigma\cdot\mathbf{\Sigma}$.

2 Global quantities

- The partition function reads [2]:

$$\text{Classical:} \qquad Z_{\rm cl} = \int \frac{d^3p\, d^3x}{(2\pi\hbar)^3}\rho = \frac{1}{\omega(\omega^2-\Omega^2)(\beta\hbar)^3}$$

$$\text{Quantum:} \qquad Z_{\rm q} = \mathrm{Tr}[\rho] = \frac{e^{\frac{3}{2}\beta\hbar\omega}\sinh\left[(s+\frac{1}{2})\beta\hbar\Omega_\Sigma\right]}{(e^{\beta\hbar(\omega+\Omega)}-1)(e^{\beta\hbar\omega}-1)(e^{\beta\hbar(\omega-\Omega)}-1)\sinh(\frac{1}{2}\beta\hbar\Omega_\Sigma)}$$

where the trace is taken over the main (n), orbital (l), magnetic (m) and spin (m_s) quantum numbers:

$$\mathrm{Tr}[\rho] = \sum_{n,l,m,m_s}\langle n,l,m,m_s|\rho|n,l,m,m_s\rangle = \sum_{n=0}^{\infty}\sum_{l=0}^{n}\sum_{m=-l}^{l}\sum_{m_s=-s}^{s} e^{-\beta\hbar[\omega(n+\frac{3}{2})-m\Omega-m_s\Omega_\Sigma]}.$$

- The total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{\Sigma}$ is comprised of the orbital part,

$$L_{\rm cl} = \frac{2\Omega}{\beta(\omega^2-\Omega^2)}, \qquad L_q = \frac{\hbar\sinh(\beta\hbar\Omega)}{\cosh(\beta\hbar\omega)-\cosh(\beta\hbar\Omega)}$$

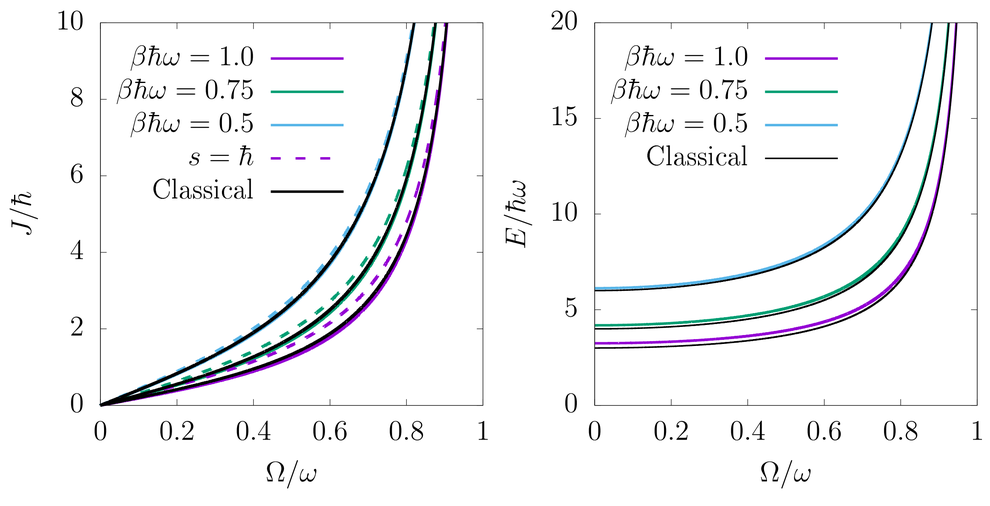
and spin part:

$$\Sigma_{\rm cl} = 0, \quad \Sigma_q = \hbar\left[\left(s+\frac{1}{2}\right)\coth\left(\left(s+\frac{1}{2}\right)\beta\hbar\Omega_\Sigma\right) - \frac{1}{2}\coth\left(\frac{\beta\hbar\Omega_\Sigma}{2}\right)\right].$$

- The average energy evaluates to:

$$E_{\rm cl} = \frac{3\omega^2-\Omega^2}{\beta(\omega^2-\Omega^2)}, \qquad E_q = \hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1} + \frac{1}{e^{\beta\hbar(\omega+\Omega)}-1} + \frac{1}{e^{\beta\hbar(\omega-\Omega)}-1} + \frac{3}{2}\right).$$

- The figures below show the dependency of J and E on $\Omega = \Omega_\Sigma$ for various temperatures:



3 Density of observable

- We introduce the position-dependent partition function as follows:

$$Z(\mathbf{x}) = \mathrm{Tr}\left(|\mathbf{x}\rangle\langle\mathbf{x}|\,\rho\right) = \sum_{n,l,m,m_s}\langle n,l,m,m_s|\mathbf{x}\rangle\langle\mathbf{x}|\rho|n,l,m,m_s\rangle,$$

where $|n,l,m,m_s\rangle$ is the usual basis and $|\mathbf{x}\rangle = |r,\theta,\varphi\rangle$ is the coordinate basis in spherical coordinates. The partition function can be expanded as

$$Z(\mathbf{x}) = \sum_{n=0}^{\infty} e^{-\beta E_n}\sum_{l,m}|\psi_{nlm}(r,\theta,\phi)|^2 e^{m\beta\hbar\Omega}\sum_{m_s=-s}^{s} e^{m_s\beta\hbar\Omega_\Sigma}$$

with the spherical eigenfunctions given by $\left[\zeta = \boldsymbol{\xi}^2, \boldsymbol{\xi} = \sqrt{\frac{m\omega}{\hbar}}\mathbf{r}\right]$

$$\psi_{nlm}(r,\theta,\phi) = \sqrt{\frac{2\Gamma(\frac{n-l}{2}+1)}{\Gamma(\frac{n-l}{2}+l+\frac{3}{2})}\left(\frac{m\omega}{\hbar}\right)^{l+\frac{3}{2}}}e^{-\zeta/2}r^l L^{(l+1/2)}_{(n-l)/2}(\zeta)Y_{lm}(\theta,\varphi).$$

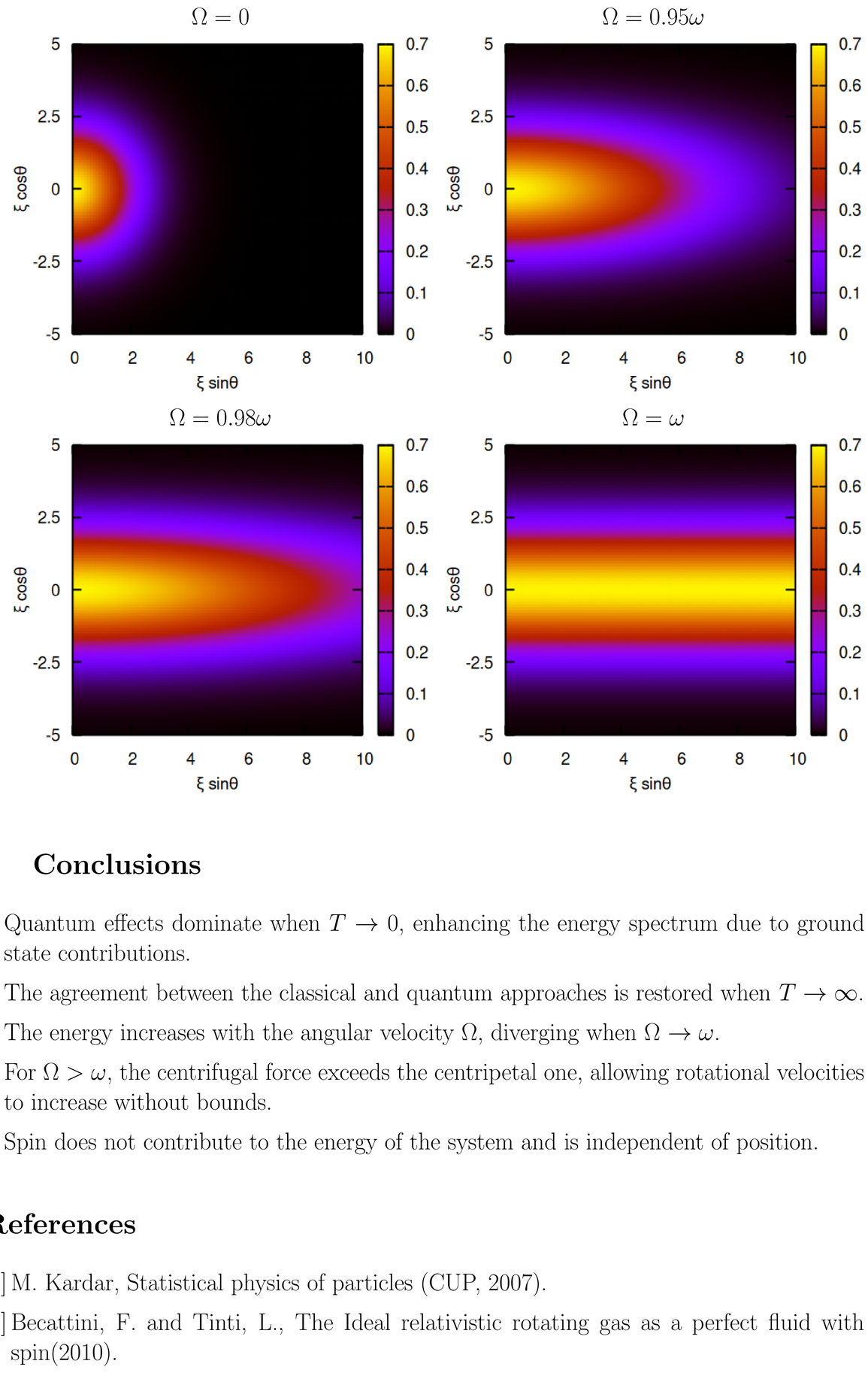
- Solving for Z one gets

$$Z(\boldsymbol{\xi}) = \frac{\sinh\left((s+\frac{1}{2})\beta\hbar\Omega_\Sigma\right)}{\sinh(\frac{1}{2}\beta\hbar\Omega_\Sigma)} \times \Lambda \times \sqrt{\frac{x}{2\pi}}e^x\left\{1 + 2x\sqrt{\lambda-1}\int_0^1 d\tau\,(1-\tau)e^{2x\tau(\lambda-1)-2x\tau^2\lambda} \times\left[\sqrt{\lambda-1}I_0(2x\tau(1-\tau)\sqrt{\lambda^2-1}) + \sqrt{\lambda+1}I_1(2x\tau(1-\tau)\sqrt{\lambda^2-1})\right]\right\},$$

where

$$\Lambda = \frac{\xi^{-1}\exp\left[-\xi^2\frac{e^{-\beta\hbar\omega}}{\sinh\beta\hbar\omega}\right]}{2\pi\sinh(\beta\hbar\omega)}, \quad x = \frac{\boldsymbol{\xi}^2}{\sinh(\beta\hbar\omega)}, \quad \lambda = 1 + 2\sin^2\theta\sinh^2(\beta\hbar\Omega/2).$$

- The figures below show the 2D representations of $Z(\boldsymbol{\xi})$ (color box), with $\Omega \in \{0, 0.95\omega, 0.98\omega, \omega\}$ and $\beta\hbar\omega = 0.5$, while $s = 1$.



4 Conclusions

- Quantum effects dominate when $T \to 0$, enhancing the energy spectrum due to ground state contributions.
- The agreement between the classical and quantum approaches is restored when $T \to \infty$.
- The energy increases with the angular velocity Ω, diverging when $\Omega \to \omega$.
- For $\Omega > \omega$, the centrifugal force exceeds the centripetal one, allowing rotational velocities to increase without bounds.
- Spin does not contribute to the energy of the system and is independent of position.

References

[1] M. Kardar, Statistical physics of particles (CUP, 2007).

[2] Becattini, F. and Tinti, L., The Ideal relativistic rotating gas as a perfect fluid with spin(2010).