Describing the ground state of quantum systems through statistical mechanics

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Talk Outline

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Introduction

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We observe that, for certain classes of quantum systems, taking different intensities of the interaction between particles of the system corresponds to taking different occupation probabilities for non-interacting microstates energy levels.

With this observation we can define an analog of the absolute temperature scale in such a manner that it is possible to make a thermodynamic interpretation for the interaction in the ground-state of quantum systems.

Formalism

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- *T* is the dimensionless interaction parameter.
- V is positively defined.
- The energy is a concave function of *T*.
- The eigenstates of the Hamiltonian in the absence of interaction ($T = 0$) are just the non-interacting states $|\phi_i>$, whose respective energy eigenvalues, $E_i(0)$ are defined through the relation $H_0|\phi_i> = E_i(0)|\phi_i>$.

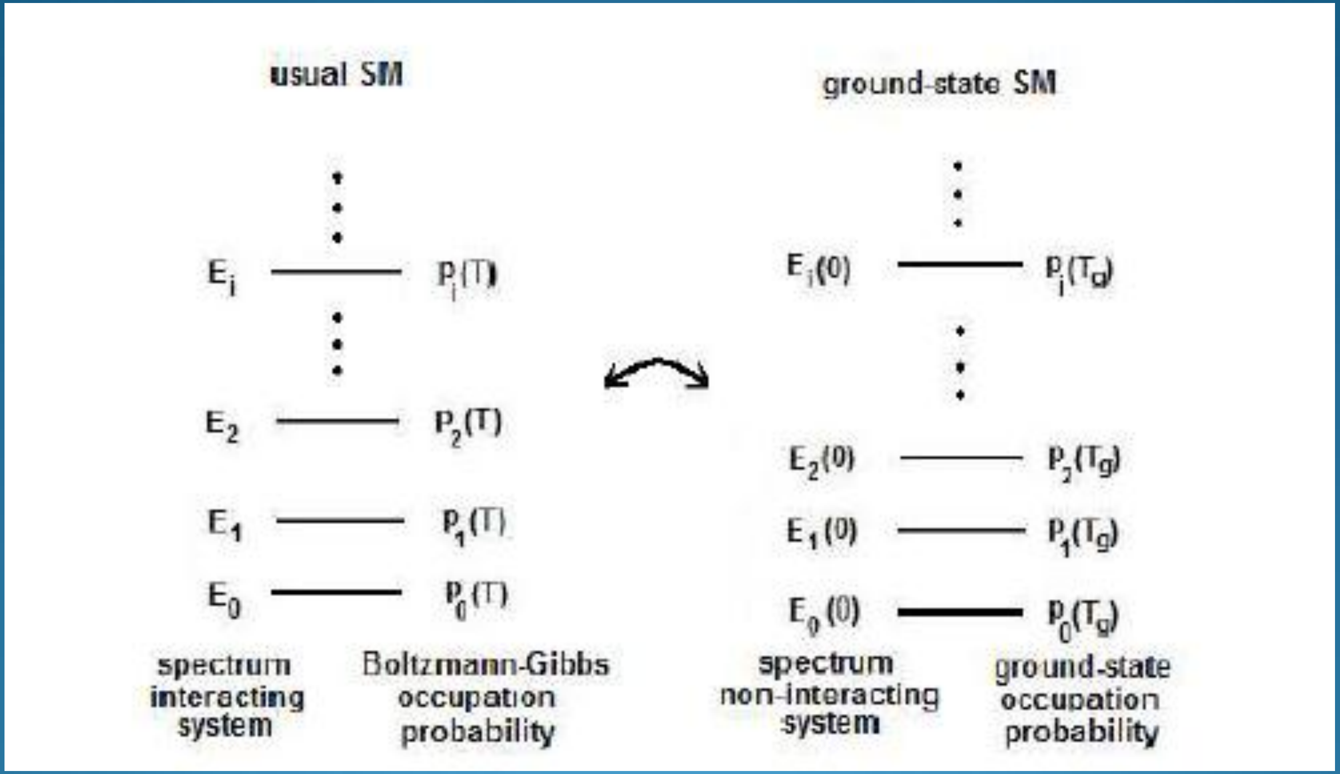
The ground-state $|\psi_0\rangle$ can be expanded in terms of the non-interacting states states $|\phi_i\rangle$ as

$$|\psi_0\rangle = \sum_i a_i(T)|\phi_i\rangle,$$

The coeficients $a_i(T) = \langle \psi_0 | \phi_i \rangle$ and $p_i(T)=|a_i(T)|^2$

For the non-interacting case $T = 0$ the system has the lowest energy $E_0(0)$ and $p_i(0) = \delta_{io}$. If $T > 0$, like a thermal energy, the interaction favors other energy levels of the non-interacting case.

Only the non-interacting microscopic states are used to compute the *thermodynamic* properties. This enables us to define an analog of the absolute temperature scale, called ground-state temperature, as $T_g = T/k$, where k is a constant measured in Kelvins^{-1}.



usual SM
ground-state SM
E_i
P_i(T)
E_2
P_2(T)
E_1
P_1(T)
E_0
P_0(T)
spectrum
interacting
system
Boltzmann-Gibbs
occupation
probability
E_i(0)
P_i(T_g)
E_2(0)
P_2(T_g)
E_1(0)
P_1(T_g)
E_0(0)
P_0(T_g)
spectrum
non-interacting
system
ground-state
occupation
probability

We can introduce a so-called ground-state thermodynamics, defining the ground-state internal energy, ground-state free energy and ground-state entropy, respectively, as:

$$U(T_g) = \langle \hat{H}_0(T_g) \rangle = \sum_i p_i(T_g) E_i(0),$$

$$F(T_g) = \langle \hat{H}(T_g) \rangle - kT_g \langle \hat{V}(0) \rangle,$$

$$S(T_g) = k(\langle \hat{V}(0) \rangle - \langle \hat{V}(T_g) \rangle).$$

We can verify that the ground-state thermodynamics precisely satisfies the standard thermodynamics relation for the Helmholtz free energy

$$F(T_g) = U(T_g) - T_g\, S(T_g).$$

the heat capacity

$$C(T_g) = T_g \frac{dS(T_g)}{dT_g} = -T_g \frac{d^2 F(T_g)}{dT_g^2}.$$

Applications

Let us study two exact solvable problems based on the Hubbard model

$$\hat{H} = -t \sum_{\langle ij \rangle \alpha} \hat{c}^{\dagger}_{i\alpha} \hat{c}_{j\alpha} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},$$

We define $T_g = U/kt$

1) Two electrons in two sites

$$E_0(U) = -\frac{1}{2}(U - \sqrt{U^2 + (4t)^2}),$$

$$|\psi_0\rangle = a_-|\phi_-\rangle + a_+|\phi_+\rangle$$

$$a_+ = 2t/\sqrt{(2\sqrt{U^2 + (4t)^2} - U)\sqrt{U^2 + (4t)^2}}.$$

$$a_- = \sqrt{1 - a_+^2}$$

$$F(T_g) = -\frac{1}{2}\sqrt{T_g^2 + 16},$$

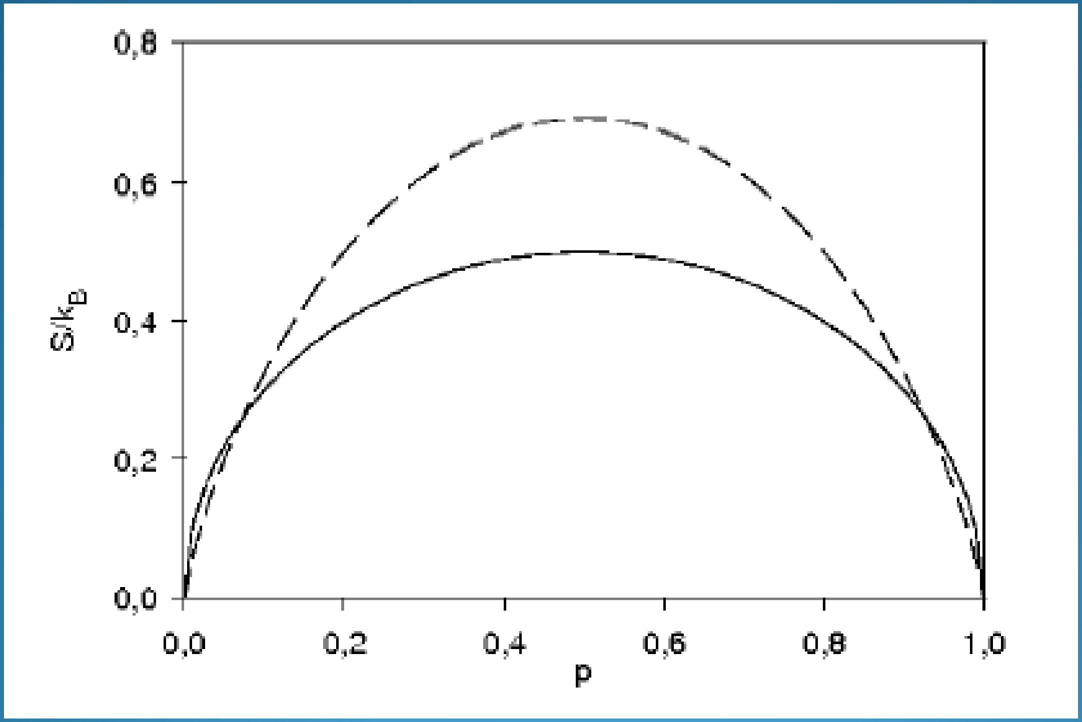
$$S(T_g) = \frac{T_g}{2\sqrt{T_g^2 + 16}},$$

$$U(T_g) = -\frac{8}{\sqrt{T_g^2 + 16}},$$

$$C(T_g) = \frac{8T_g}{2(T_g^2 + 16)^{3/2}}.$$

$$p_\pm(T_g) = \frac{1}{2} \mp \frac{2}{\sqrt{T_g^2 + 16}}.$$

$$S(p) = \sqrt{p_+ p_-},$$



Boltzmann-Gibbs (dashed line) - 2 states (full line).

2) half-filled band of the Hubbard model for the one-dimensional case in the thermodynamic limit

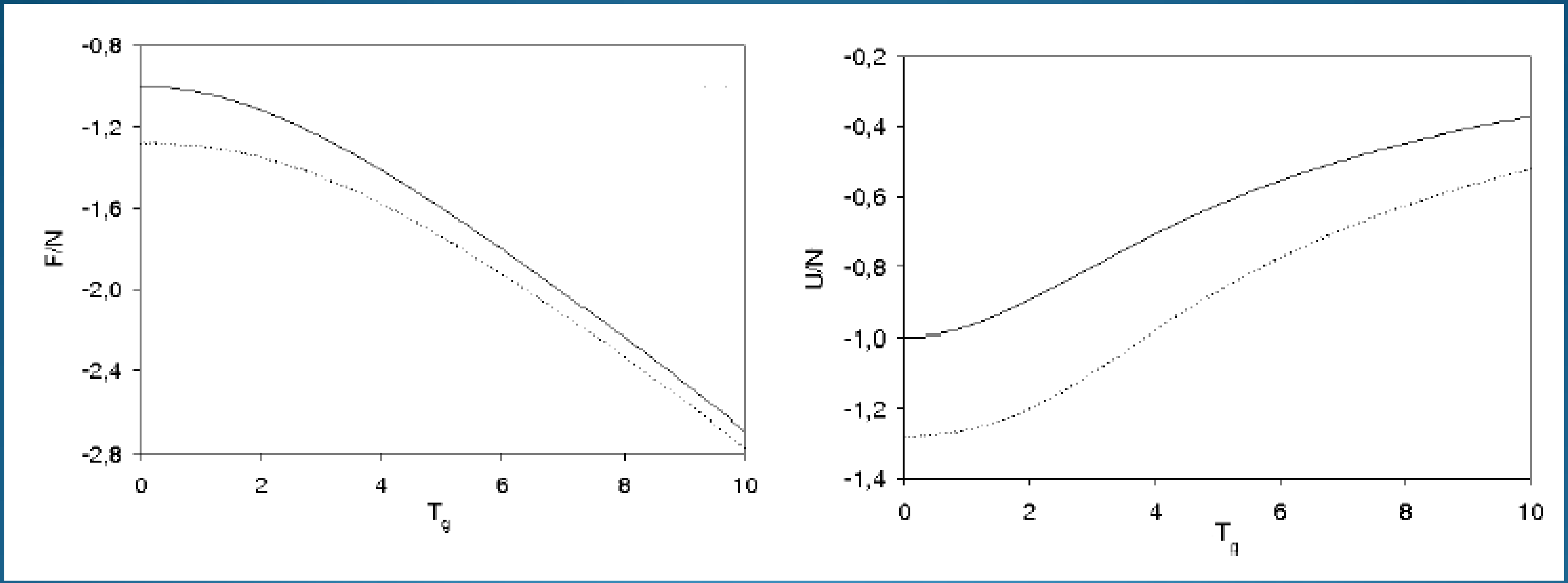
$$F(T_g)/N = -\frac{T_g}{4} - 4\int_0^\infty \frac{J_0(w)J_1(w)dw}{w[1+\exp(wT_g/2)]},$$

$$S(T_g)/N = \frac{1}{4} - \frac{1}{2}\int_0^\infty \frac{J_0(w)J_1(w)dw}{\cosh^2(wT_g/4)},$$

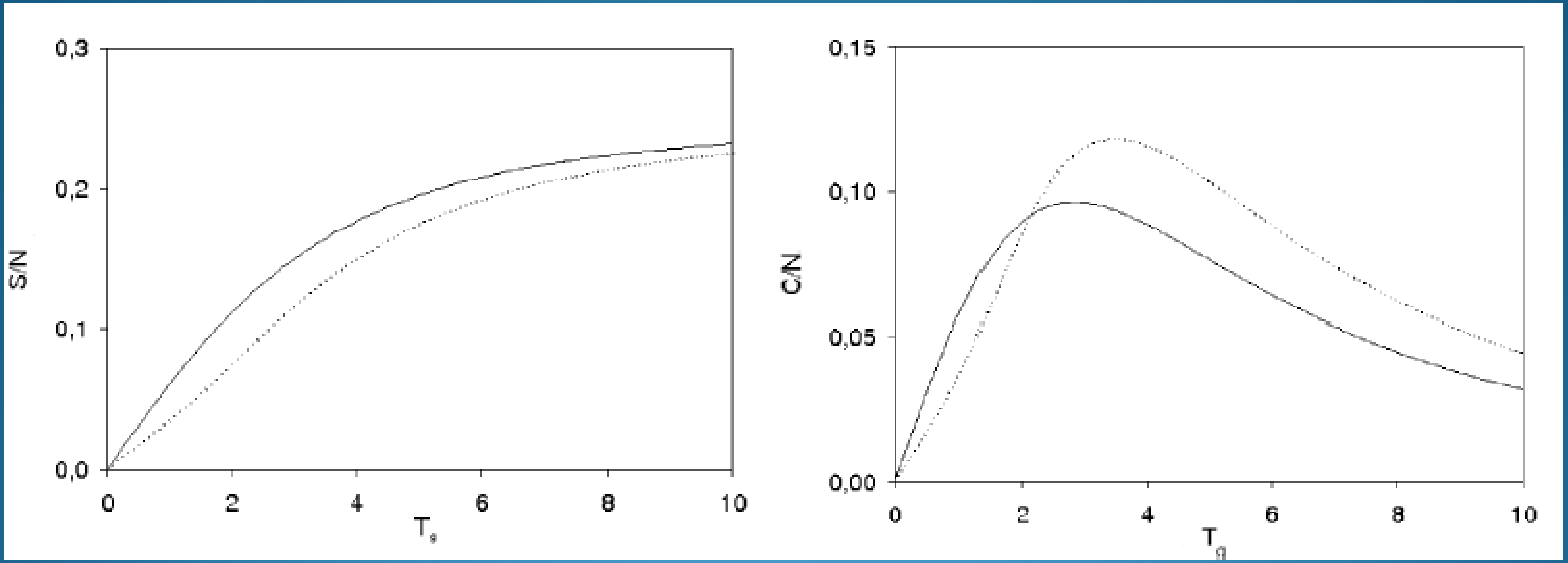
$$U(T_g)/N = -\int_0^\infty \frac{J_0(w)J_1(w)f(w,T_g)dw}{w[1+\exp(wT_g/2)]^2},$$

$$f(w,T_g) = [4 + (4 + wT_g/2)\exp(wT_g/2)]$$

$$C(T_g)/N = \frac{T_g}{4}\int_0^\infty \frac{wJ_0(w)J_1(w)\sinh(wT_g/4)dw}{\cosh^3(wT_g/4)}.$$



The full line represents the case $N = 2$ and two electrons, while the dotted line represents the half-filled band for the one-dimensional case in the thermodynamic limit ($N \rightarrow \infty$)



S/N
0,3
0,2
0,1
0,0
0
2
4
6
8
10
T_g
C/N
0,15
0,10
0,05
0,00
0
2
4
6
8
10
T_g

Conclusions

We present an approach to solve problems of quantum mechanics using concepts of statistical mechanics.

We can consider that taking different ground-state temperatures T_g, i.e, different values of the interaction parameter, the particles of the system fall into non-interacting microstates, corresponding to different occupation probabilities for these energy levels.

We found that the functional form of the ground-state entropy depends on the particular quantum system.

The ideas presented here can eventually provide a mechanism for new approximation methods, such as the usage of the geometric average of the quantum states probability in the high dimensional limit for the Hubbard model.

We can envisage in further works the study of the possibility that many different systems may fall into some basic classes of the ground-state entropy.