BÖLÜM 8

KUANTUM İSTATİSTİK MEKANİĞİ

Doğadaki tüm sistemler QM'ne uyar. QM de ise bir sist. in gözlenebilirleri Hilbert uzayında opere eden Hermitsel bir op. ile ilintilidir.

göz. karşılık gelen op.

$$X|q\rangle = x|q\rangle$$

kon. önek.

$$|\psi\rangle \in \mathcal{H}$$

$$\langle q|\psi\rangle = \psi(q)$$

$$\psi = \sum_n c_n \Phi_n$$

$\in \mathbb{C}$ $\quad c_n \equiv c_n(t)$ $\quad n \equi \{\text{Q. num.}\}$

$|c_n|^2$ olasılık.

$$\frac{(\psi, \theta\psi)}{(\psi,\psi)} = \frac{\sum_{nm} (c_n, c_m)(\Phi_n, \theta \Phi_m)}{\sum_n (c_n, c_n)}$$

Skaler pr

Gerçek bir ölçüm için de zaman ortalamasına ihtiyaç vardır.

$$\langle \theta \rangle = \frac{\sum_{nm} \overline{(c_n, c_m)} (\Phi_n, \theta \Phi_m)}{\sum_n \overline{(c_n, c_n)}}$$

N-parçacıklı E enerjili bir sist.

Sist. in enerjisi $E < E_n < E + \Delta$ arasında bulunur.

Ham. tanımı $\mathcal{H}$

$$\mathcal{H}\Phi_n = E_n \Phi_n$$

1. Eşit önsel postülası.

$$\overline{(c_n, c_n)} = \begin{cases} 1 & E < E_n < E+\Delta \\ 0 & \text{sınır dışında} \end{cases}$$

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2. Gelişi güzel fazlar postülası :

$$(C_n, C_m) = 0 \qquad n \neq m$$ gibiyin etkisi ihmal

bunların neticesinde $\Psi = \sum_n b_n \Phi_n$

$$|b_n|^2 = \begin{cases} 1 & E < E_n < E + \Delta \\ 0 & \text{dışında} \end{cases}$$

$$\langle \Theta \rangle = \frac{\sum_n |b_n|^2 (\Phi_n, \Theta \Phi_n)}{\sum_n |b_n|^2}$$

Sist. i. bir durum. Bundan ∞ tane olarak bir istatistik topluluk (Gibbsian'ın QM sel genellemesi) oluşturuyor

yoğ. matrisi $\rho_{mn} = \delta_{mn} |b_n|^2 = (\Phi_n, \rho \Phi_m)$ tanım

$$\langle \Theta \rangle = \frac{\sum_n (\Phi_n, \Theta \rho \Phi_n)}{\sum_n (\Phi_n, \rho \Phi_n)} = \frac{Tr(\rho \Theta)}{Tr(\rho)}$$

$$Tr(AB) = Tr(BA) \qquad Tr(SAS^{-1}) = Tr(A)$$

$$i\hbar \frac{\partial \rho}{\partial t} = [\mathcal{H}, \rho] \qquad \rho = \sum_n |\Phi_n\rangle |b_n|^2 \langle \Phi_n|$$

8.3. Q.İ.M de topluluklar :

mikrokanonik topluluk

$$\rho_{mn} = \delta_{mn} |b_n|^2$$

$$|b_n|^2 = \begin{cases} \text{sbt} & E < E_n < E + \Delta \\ 0 & \text{dışında} \end{cases}$$

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$$\exists \ \rho = \sum_n |\Psi_n\rangle\langle\Phi_n|$$

$$\mathrm{Tr}(\rho) = \sum_n \rho_{nn} \equiv \Gamma(E)$$

$$S(E,V) = k \log \Gamma(E)$$

Kanonik topluluk:

$$\frac{1}{N!\,h^{3N}} \int dq\, dp \rightarrow \sum_n$$

$$\rho_{mn} = \delta_{mn}\, e^{-\beta E_n} \qquad Q_N = \mathrm{Tr}\,\rho = \sum_n e^{-\beta E_n} = \mathrm{Tr}\, e^{-\beta H}$$

$$\langle \Theta \rangle = \frac{\mathrm{Tr}(\Theta e^{-\beta H})}{Q_N}$$

Büyük kanonik topluluk.

$$\mathcal{Z}(z,V,T) = \sum_N z^N Q_N$$

$$\langle \Theta \rangle = \frac{1}{\mathcal{Z}} \sum z^N \langle Q_N \rangle$$

$$\mathcal{Z}(z,V,T) = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right)$$

$$\langle \Theta \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}\left(\Theta\, e^{-\beta(H-\mu N)}\right)$$

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8.7 İdeal Gazlar MKT

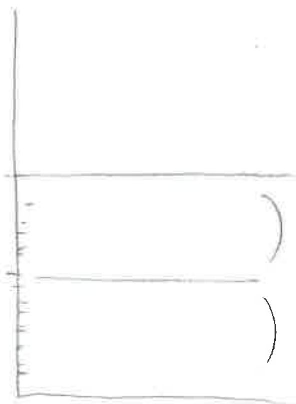
$$\epsilon_i = \sum_i \frac{p_i^2}{2m} \quad \text{Spini gözönüne almayalım.}$$

$$\epsilon_p = \frac{\vec{p}^2}{2m} \qquad p_i^2 = \vec{p}_i \cdot \vec{p}_i$$

parçacık sist. için top. enerji $\quad E = \sum_{\vec{p}} n_{\vec{p}}\, \epsilon_{\vec{p}} \qquad N = \sum_{\vec{p}} n_{\vec{p}}$

$$n_{\vec{p}} = \begin{cases} 0, 1, 2, \dots & \text{Bozon} \\ 0, 1 & \text{Fermiyon} \end{cases}$$

Bir de Boltzman ist. ne uyan parçacıklar vardı.



g_i, n_i

g_2, n_2

$g_1, n_1 \to$ parçacık sayısı

En. düzeyi sayısı

İlgili sayının karşı gelen sist. in durumların sayısı

$W\{n_i\}$ diyor

$$\sum_{\{n_i\}} N\{n_i\} = \Gamma(E) \quad \text{I}$$

$$E = \sum_i \epsilon_i n_i$$

$$N = \sum_i n_i$$

koşulları altında ifadesini ext. yapacağız.

n_i parçacığı (i. hücreye atanmış) dağıtmanın yollarının sayısı (g_i düzey için)

Bozonlar :

$g_i - 1$ bölme var.

(g_i, n_i, ϵ_i) ordul

$$\frac{(n_i + (g_i - 1))!}{n_i!\,(g_i - 1)!}$$

Sayıda n_i parçacığı dağıtabiliriz

$$\frac{(2+1)!}{2!\,1!} = 3$$

(2), 2, ϵ_1, ϵ_2

(1) ϵ_1 (1, 2, ϵ_1, ϵ_2)

n_1	0	1	0	2	1	0	3	2	1	0
n_2	0	0	1	0	1	2	0	1	2	3
N	0	1	1	2	2	2	3	3	3	3

$\underbrace{0}_{1}\ \underbrace{1\ 1}_{2}\ \underbrace{2\ 2\ 2}_{3}\ \underbrace{3\ 3\ 3\ 3}_{4}$

Fermiyonlar $\qquad N\{n_i\} = \prod_i \frac{g_i!}{n_i!\,(g_i-n_i)!} =$

$i=2 \longrightarrow \frac{g_1!}{n_1!\,(g_1-n_1)!}\,\frac{g_2!}{n_2!\,(g_2-n_2)!}$

$\left.\begin{matrix} g_1=g_2=2 \\ n_1=n_2=2 \end{matrix}\right) \to \frac{(2!)^2}{(2!)^2\,(0!)^2} = 1$ $\quad$ #

Boltzman Gaz. $\qquad w_i = \frac{N!\; g_i!}{\prod_i n_i}$

$W\{n_i\} = \frac{1}{N!}\, w_i$

#

$\delta\left[\ln W - \beta E - \alpha N\right] = 0$ ekstremuma gerekir

$\bar{n}_i = \frac{g_i}{z^{-1} e^{\beta \epsilon_i} - 1}$

$S = k \ln W\{n_i\} \qquad \overline{n_i^2} - \bar{n}_i^2 \ll \bar{n}_{n_i}^2$

$N = z \sum_i g_i\, e^{-\beta \epsilon_i} \qquad E = \sum g_i \epsilon_i e^{-\beta \epsilon_i} = \frac{3}{2} NkT$

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aynı şeyi BKT de yapmak mümkün:

$Q_N = \sum g\{n_p\}\, e^{-\beta E\{n_p\}}$

$g\{n_p\} = \begin{cases} 1 & \text{Bose\_Fermi} \\ \frac{1}{N!}\,\frac{N!}{\prod_p n_p!} & \text{Boltzmann} \end{cases}$

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8.1.

$$|\psi\rangle = A \begin{pmatrix} 1 \\ 0 \end{pmatrix} + B \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle \psi | = A^* (1 \; 0) + B^* (0, 1)$$

$$\rho = \sum_n |\Phi_n\rangle |b_n|^2 \langle \Phi_n| = |\psi\rangle\langle\Psi|$$

$$= |A|^2 \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + |B|^2 \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$+ AB^* \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + A^* B \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} |A|^2 & AB^* \\ A^* B & |B|^2 \end{pmatrix}$$

prob. m kütleli serbest parçacık için ρ'nun koordinat gösterimi:

$$H = p^2/2m \qquad H\Phi_E = E\Phi_E \qquad \Phi_E = C e^{i\vec{k}\cdot\vec{r}}$$

L^3 normalizasyonu yapalım. $|\vec{k}| = \frac{2\pi}{L} (n_x \; n_y \; n_z)$

$$\rho = e^{-\beta H}/Q$$

$$\langle r|\rho|r'\rangle = ?$$

$$\rho = \frac{1}{Q} \sum_E |\Phi_E\rangle e^{-\beta E} \langle \Phi_E|$$

$$E = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

BS K

$$\langle r|\rho|r'\rangle = \frac{1}{Q}\sum_E \varphi_E(\vec r)\, e^{-\beta E}\, \varphi_E^*(\vec r\,') \qquad c = \frac{1}{\sqrt{L^3}}$$

$$= \frac{1}{L^3}\sum e^{i\vec k\cdot(\vec r-\vec r\,')} e^{-\beta E} = \frac{1}{L^3}\sum e^{i\vec k\cdot(\vec r-\vec r\,')} e^{-\frac{\hbar^2}{2m}\frac{4\pi^2}{L^2}(n_x^2+n_y^2+n_z^2)}$$

$$\langle x|\rho|x'\rangle = \frac{1}{L}\sum_{n_x=-\infty}^{+\infty} e^{i\frac{2\pi}{L}n_x(x-x') - \frac{\hbar^2}{2m}\frac{4\pi^2}{L^2}n_x^2}$$

$$L\to\infty \qquad \sum_{n=-\infty}^{+\infty}\frac{1}{L} \to \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk_x$$

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk_x\, e^{ik_x(x-x') - \frac{\hbar^2 k_x^2}{2m}}$$

$$= \left(m/2\pi\hbar^2\beta\right)^{1/2} e^{-\frac{m}{2\beta\hbar^2}(x-x')^2}$$

$$\langle r|\rho|r'\rangle = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} e^{-\frac{m}{2\beta\hbar^2}(\vec r-\vec r\,')^2}$$

problem: magnetik alanda tek elektron

$$\vec S = \frac{\hbar}{2}\vec\sigma \qquad \mu_B = \frac{e\hbar}{2mc} \qquad \hat z \parallel \vec B \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$H = -\mu_B\, \vec\sigma\cdot\vec B = -\mu_B B \sigma_z$$

$$\rho = e^{-\beta H}/\mathrm{Tr}\,\rho$$

$$e^{-\beta H} = e^{\beta\mu_B B\sigma_z} = e^{a\sigma_z} = I\,\mathrm{ch}\,a + \sigma_z\,\mathrm{sh}\,a$$

BS K

$$\rho = \frac{1}{2\,\mathrm{ch}\,a}\begin{pmatrix} \mathrm{ch}\,a + \mathrm{sh}\,a & 0 \\ 0 & \mathrm{ch}\,a - \mathrm{sh}\,a \end{pmatrix}$$

$$= \frac{1}{2\,\mathrm{ch}\,a}\begin{pmatrix} e^{a} & 0 \\ 0 & e^{-a} \end{pmatrix}$$

$$\langle \sigma_z \rangle = \mathrm{Tr}\,(\rho\,\sigma_z) = \frac{1}{2\,\mathrm{ch}\,a}\,\mathrm{Tr}\left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} e^{a} & 0 \\ 0 & e^{-a} \end{pmatrix}\right]$$

$$= \mathrm{th}\,a$$

8.5 Harmonik salınıcı için yoğunluk matrisi

$$\mathcal{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2} m\,\omega^2 q^2 \qquad E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$n = 0, 1, 2, \ldots$$

$$\langle q | e^{-\beta \mathcal{H}} | q' \rangle = \sum_n e^{-\beta E_n}\, \varphi_n(q)\, \varphi_n^*(q')$$

$$\varphi_n(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{H_n(x)}{(2^n n!)^{1/2}}\, e^{-x^2/2} \qquad x = \left(\frac{m\omega}{\hbar}\right)^{1/2} q$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-\frac{1}{2}(x^2+x'^2)} \sum_{n=-\infty}^{+\infty} e^{-\beta(n+\frac{1}{2})\hbar\omega}\, \frac{H_n(x)\,H_n(x')}{2^n n!}$$

$$= \left(\frac{m\omega}{2\pi\hbar\,\mathrm{sh}\,\beta\hbar\omega}\right)^{1/2} e^{-\frac{m\omega}{4\hbar}\left[(q+q')^2\,\mathrm{th}\,\frac{\beta\hbar\omega}{2} + (q-q')^2\,\mathrm{cth}\,\frac{\beta\hbar\omega}{2}\right]}$$

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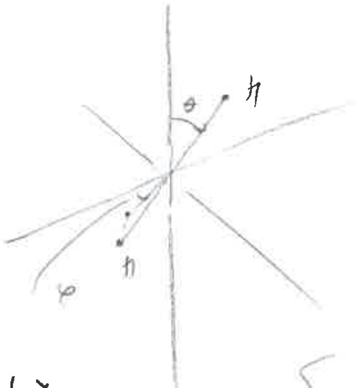
$$\mathrm{Tr}\, e^{-\beta H} = \left(\frac{m\omega}{2\pi\hbar\, \mathrm{sh}\, \beta\hbar\omega} \right) \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar} q^2 \,\mathrm{th}\, \frac{\beta\hbar\omega}{2}} dq$$

$$= \frac{1}{2\,\mathrm{sh}\left(\frac{\beta\hbar\omega}{2}\right)} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} \to Q_1$$

$$\langle q|\rho|q\rangle = \left[\frac{m\omega}{\pi\hbar} \tanh \frac{\beta\hbar\omega}{2} \right]^{1/2} e^{-\frac{m\omega}{\hbar} q^2 \,\mathrm{th}\, \frac{\beta\hbar\omega}{2}}$$

$\beta\hbar\omega \ll 1$ klasik limit $\quad \langle q|\rho|q\rangle \simeq \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} e^{-m\omega q^2/\hbar}$

§ 6. H_2 singlet → para



$$h = \frac{p_\theta^2}{2I} + \frac{p_\varphi^2}{2I \sin^2\theta} \qquad I = \frac{1}{2} m r_0^2$$

$$\epsilon_l = \frac{\hbar^2}{2I} l(l+1) \begin{cases} l \text{ tek orto} \\ l \text{ çift para} \end{cases} \quad 0, 1, 2, \ldots$$

$g_l = 2l+1$ dejenere.

$$Q = \sum_l g_l\, e^{-\beta\epsilon_l} = \sum_{l=0}^{\infty} (2l+1)\, e^{-\frac{\hbar^2}{2IkT} l(l+1)}$$

$$\frac{\hbar^2}{2Ik} = \Theta_r$$

$$Q = \sum_l (2l+1)\, e^{-\frac{\Theta_r}{T} l(l+1)}$$

$$\sum_n f(n) = \int_0^\infty dx\, f(x) + \frac{1}{2} f(0) - \frac{1}{12} f'(0) + \frac{1}{720} f''(0) \ldots$$

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(a) $\Theta_r \ll T$

$$Q(T) = \frac{T}{\Theta_r} + \frac{1}{3} + \frac{1}{15}\frac{\Theta_r}{T} + \frac{4}{315}\left(\frac{\Theta_r}{T}\right)^2$$

$$\simeq \frac{T}{\Theta_r}$$

(b) $\Theta_r \gg T$

$$Q(T) = 1 + 3e^{-2\Theta_r/T} + 5e^{-6\Theta_r/T}$$

$S=0$ singlet → para $\quad \epsilon = \frac{\hbar^2}{2I} l(l+1) \quad l = 0, 2, \ldots$

$S=1$ triplet → ortho $\quad$ " $\quad l = 1, 3, 5, \ldots$

$$Q_p = \sum_{l=0,2} (2l+1)\, e^{-\Theta_r l(l+1)/T}$$

$$Q_{or} = \sum_{l=1,3} (2l+1)\, e^{-\Theta_r l(l+1)/T}$$

$$\frac{N_{or}}{N_{par}} = \frac{Q_{or}}{Q_{par}} = \frac{3\sum_{l\ \mathrm{odd}} (2l+1)\, e^{-\Theta_r l(l+1)/T}}{\sum_{l\ \mathrm{even}} (2l+1)\, e^{-\Theta_r l(l+1)/T}}$$

(a) $T \to 0 \qquad \frac{N_o}{N_p} = \frac{9e^{-2\Theta_r/T}}{1} \to 0$

(b) $T \gg \Theta_r \qquad \frac{N_o}{N_p} \simeq 3$

BS K