Assignments to Condensed Matter Theory I
Sheet 4

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sheet online: http://www-MCG.uni-R.de/teaching/

Problem set: Spin statistics and finite temperatures

In the real world we never encounter zero temperature. Hence we will often need to use statistical physics and thermodynamics. In classical mechanics the state of a system is defined by the position and momentum of all its degrees of freedom. For example the state of N classical particles is defined by the set of 6N coordinates $\mathbf{x}_n, \mathbf{p}_n$ with $n = 1, \ldots, N$ in the phase space Γ. The observables $O(\mathbf{x}_n, \mathbf{p}_n)$ are functions of these coordinates and their thermal averages can be written as:

$$\langle O \rangle_T = \sum_{N=0}^{\infty} \int_\Gamma \mathrm{d}\Gamma \rho(\mathbf{x}_n, \mathbf{p}_n, N) O(\mathbf{x}_n, \mathbf{p}_n)$$

where, according to the Gibbs formula, $\rho(\mathbf{x}_n, \mathbf{p}_n, N) \equiv (1/Z) \exp[-\beta(H(\mathbf{x}_n, \mathbf{p}_n) - \mu N)]$, $\beta = \frac{1}{k_B T}$ and $\mathrm{d}\Gamma \equiv \prod_{n=1}^{N} \mathrm{d}\mathbf{x}_n \mathrm{d}\mathbf{p}_n$. Z is the grancanonical partition function:

$$Z = \sum_{N=0}^{\infty} \int_\Gamma \mathrm{d}\Gamma \exp[-\beta(H(\mathbf{x}_n, \mathbf{p}_n) - \mu N)]$$

The quantum mechanical version of the thermal average is:

$$\langle O \rangle_T = \sum_{N=0}^{\infty} \mathrm{Tr}_N \{\hat{\rho} \hat{O}\}$$

where the operator $\hat{\rho}$ is defined as:

$$\hat{\rho} = (1/Z) \exp[-\beta(\hat{H} - \mu \hat{N})]$$

and the trace Tr_N is taken only with respect to states with N number of particles. The grancanonical partition function, in the quantum version, reads:

$$Z = \sum_{N=0}^{\infty} \mathrm{Tr}_N \{\exp[-\beta(\hat{H} - \mu \hat{N})]\}$$

4.1. Many (non-interacting) bosons

Let us consider the Hamiltonian for non-interacting bosons:

$$H_\mathrm{B} = \sum_\lambda \hbar\omega_\lambda \left(b_\lambda^\dagger b_\lambda + \frac{1}{2} \right) \tag{1}$$

where the quantum number λ completely defines the single particle state. For example in the case of a system of phonons $\lambda = (\mathbf{q}, m)$ where $\mathbf{q}$ is the momentum and m the branch index. The chemical potential μ is taken to be lower than the lowest boson energy and independent from the temperature.

(a) Calculate the grancanonical partition function Z for this system.

(b) What is the average number of bosons in the state defined by the quantum number λ? This is called Bose-Einstein distribution n_{BE}.

(c) Plot $n_{\mathrm{BE}}(\omega_\lambda, T, \mu)$ vs. ω_λ for different temperatures.

(d) What is the average energy U of the system?
`Hint:` $U = -\frac{\partial}{\partial \beta} \ln Z + \frac{\mu}{\beta} \frac{\partial}{\partial \mu} \ln Z$.

(e) **[Kür]** Calculate the specific heat $c_V = \frac{\partial U}{\partial T}$ using the Einstein model (i.e. only one branch with dispersion $\omega(\mathbf{q}) = \omega_0$).

(f) **[Kür]** Calculate the specific heat c_V at low temperatures for phonons with linear dispersion relation $\omega(\mathbf{q}) = v\|\mathbf{q}\|$ in 1D, 2D, 3D.
`Hint:` It is not (so) difficult to show that:

$$c_V = N k_B \int_0^\infty \mathrm{d}\omega \left(\frac{\hbar\omega}{2k_B T} \right)^2 \frac{DOS(\omega)}{\sinh^2(\hbar\omega/2k_B T)}$$

4.2. Many (non-interacting) fermions

Let us now consider the Hamiltonian for non-interacting fermions:

$$H_{\mathrm{F}} = \sum_\lambda \epsilon_\lambda c_\lambda^\dagger c_\lambda \tag{2}$$

where λ is a good quantum number for single particle states.

(a) Calculate the grancanonical partition function Z for this system.
`Hint:` Remember that for Fermions the Pauli exclusion principle holds. Formally $\{c^\dagger, c^\dagger\} = 0$ which implies that a single particle state can never be occupied by more than one fermion.

(b) Calculate the average number of fermions in the state defined by the quantum number λ. You just rediscover the Fermi-Dirac distribution n_{FD}.

(c) Plot $n_{\mathrm{FD}}(\epsilon_\lambda, T, \mu)$ vs. ϵ_λ for different temperatures.

(d) What is the average energy of the system?

Solutions of the exercises in the Sheet 4 of QTKM 1

4-1

a) $$Z = \sum_{N=0}^{\infty} Tr_N \left\{ \exp\left[-\beta(\hat{H} - \mu\hat{N})\right]\right\}$$

$\hat{H}$ is the Hamilton operator, in II quantization it can be written as:

$$H = \sum_\lambda \hbar\omega_\lambda \left(a_\lambda^+ a_\lambda + \frac{1}{2}\right)$$
$$N = \sum_\lambda a_\lambda^+ a_\lambda$$

The Trace Tr_N is taken over all possible states with N particles. A generic bosonic state with N particles reads:

$N = 1$ $\qquad a_\lambda^+ |0\rangle$

$N = 2$ $\qquad a_{\lambda_1}^+ a_{\lambda_2}^+ |0\rangle$ if $\lambda_1 \neq \lambda_2$ or $\frac{1}{\sqrt{2}} (a_\lambda^+)^2 |0\rangle$

⋮

N $\qquad \prod_\lambda \frac{1}{\sqrt{n_\lambda!}} (a_\lambda^+)^{n_\lambda} |0\rangle$ where $\sum_\lambda n_\lambda = N$

and we indicate it with the shortcut $|\{n_\lambda\}_N\rangle$

$$Z = \sum_{N=0}^{\infty} \sum_{\{n_\lambda\}_N} \langle \{n_\lambda\}_N | \prod_{\lambda'} \exp\left[-\beta\left(\hbar\omega_\lambda (a_{\lambda'}^+ a_{\lambda'} + \tfrac{1}{2}) - \mu a_{\lambda'}^+ a_{\lambda'}\right)\right] | \{n_\lambda\}_N\rangle$$

since $e^{A+B} = e^A \cdot e^B$ if $[A,B] = 0$

$$= \sum_{N=0}^{\infty} \sum_{\{n_\lambda\}_N} \prod_\lambda \exp\left[-\beta\left(\hbar\omega_\lambda (n_\lambda + \tfrac{1}{2}) - \mu n_\lambda\right)\right]$$

$$= \prod_\lambda \sum_{n_\lambda = 0}^{\infty} e^{-\beta \frac{\hbar\omega_\lambda}{2}} \cdot \left[e^{-\beta(\hbar\omega_\lambda - \mu)}\right]^{n_\lambda} = \prod_\lambda e^{-\beta\frac{\hbar\omega_\lambda}{2}} \frac{1}{1 - e^{-\beta(\hbar\omega_\lambda - \mu)}}$$

The most important part is to realize the validity of the identity

$$\sum_{N=0}^{\infty} \sum_{\{n_\lambda\}_N} \prod_\lambda q_\lambda^{n_\lambda} = \prod_\lambda \sum_{n_\lambda=0}^{\infty} q_\lambda^{n_\lambda} \qquad (*)$$

I think that the most intuitive way to prove this identity is to consider a generic element of the sum on the left

$$\prod_\lambda q_\lambda^{n_\lambda} \quad \text{with the configuration} \quad \{n_\lambda\}_{\bar{N}} = (n_1, n_2, n_3 \dots) : \sum_\lambda n_\lambda = N$$

and show that this is reproduced on the right

$$\left(q_1 + q_1^2 + \dots + q_1^{n_1} + \dots\right)\left(q_2 + q_2^2 + q_2^3 + \dots + q_2^{n_2} + \dots\right)\left(\quad\right) \cdot \dots$$

If one expands this last product and take only the needed element

$$q_1^{n_1} q_2^{n_2} q_3^{n_3} \dots$$

it is proven that each element of the sum on the left of $*$) appears one and only one time on the right of ($*$). The viceversa is analogous.

$$Z_B = \prod_\lambda e^{-\beta \frac{\hbar\omega_\lambda}{2}} \frac{1}{1 - e^{-\beta(\hbar\omega_\lambda - \mu)}}$$

stands for bosons

b)

$$\langle \hat{n}_\lambda \rangle = \sum_{N=1}^{\infty} Tr_N \{\rho\, b_\lambda^+ b_\lambda\} = \frac{1}{Z} \sum_{N=1}^{\infty} Tr_N \left\{ e^{-\beta(H-\mu N)}\, b_\lambda^+ b_\lambda \right\}$$

$$= \frac{1}{Z} \sum_{N=1}^{\infty} Tr_N \left\{ e^{-\beta(H-\mu N)} \left(b_\lambda^+ b_\lambda + \frac{1}{2}\right)\right\} - \frac{1}{2} = -\frac{1}{\hbar\beta} \frac{\partial}{\partial \omega_\lambda} \ln Z - \frac{1}{2}$$

$$= -\frac{1}{\hbar\beta} \frac{\partial}{\partial \omega_\lambda} \left[\ln \left(\prod_{\lambda'} e^{-\beta \frac{\hbar\omega_{\lambda'}}{2}} \frac{1}{1 - e^{-\beta(\hbar\omega_{\lambda'} - \mu)}} \right) \right] - \frac{1}{2} =$$

$\mu > \omega_{min}!$

$$= -\frac{1}{\hbar\beta} \frac{\partial}{\partial \omega_\lambda} \sum_{\lambda'} \left[-\frac{\beta\hbar\omega_{\lambda'}}{2} - \ln\left(1 - e^{-\beta(\hbar\omega_{\lambda'} - \mu)}\right) \right] - \frac{1}{2} =$$

$$= \cancel{\frac{1}{2}} + \frac{1}{\cancel{\hbar\beta}} \frac{e^{-\beta(\hbar\omega_{\lambda'} - \mu)}}{1 - e^{-\beta(\hbar\omega_\lambda - \mu)}} \cdot \cancel{\hbar\beta} - \cancel{\frac{1}{2}} = \frac{1}{e^{\beta(\hbar\omega_\lambda - \mu)} - 1}$$

$$\boxed{n_{BE}(\omega_\lambda) = \frac{1}{e^{\beta(\hbar\omega_\lambda - \mu)} - 1}}$$

BOSE EINSTEIN DISTRIBUTION

c) See attached plots

d)

$$U = -\frac{\partial}{\partial\beta} \ln Z + \mu \frac{1}{\beta}\frac{\partial}{\partial\mu} \ln Z \quad -\frac{\partial}{\partial\beta} \sum_\lambda \left[-\beta \frac{\hbar\omega_\lambda}{2} - \ln\left(1 - e^{-\beta(\hbar\omega_\lambda - \mu)}\right)\right] + \mu \frac{1}{\beta}\frac{\partial}{\partial\mu} [\quad]$$

$$= \underbrace{\sum_\lambda \frac{\hbar\omega_\lambda}{2}}_{\text{zero point energy.}} + \sum_\lambda \frac{\hbar\omega_\lambda}{e^{\beta(\hbar\omega_\lambda - \mu)} - 1}$$

μ is by definition the energy needed to add one more particle to the system. For a system of non-interacting bosons it is $\hbar\omega_{min}$ since an extra boson can always be put in the lowest energy state.

e) We said from the beginning that $\lambda = (m, q)$. In the case of single branch $\lambda = q$. We further assume that $\omega(q) = \omega_0$

$$U = \sum_q \frac{\hbar\omega_0}{2} + \sum_q \frac{\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1} = 3N\frac{\hbar\omega_0}{2} + \frac{3N\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1}$$

$$C_V = \frac{\partial U}{\partial T} = 3N\hbar\omega_0 \frac{e^{\beta\hbar\omega_0}}{\left(e^{\beta\hbar\omega_0} - 1\right)^2} \frac{\hbar\omega_0}{k_B T^2} = 3Nk_B\left(\frac{\hbar\omega_0}{k_B T}\right)^2 \frac{1}{\left(e^{\beta\hbar\omega_0/2} - e^{-\beta\hbar\omega_0/2}\right)^2}$$

In this evaluation we have considered $\mu = 0$ since the number of phonons in the system is not fixed and $\mu = \bar{U}(N+1) - \bar{U}(N)$

$$C_V = 3Nk_B\left(\frac{\hbar\omega_0}{2k_B T}\right)^2 \frac{1}{\sinh^2\left(\frac{\hbar\omega_0}{2k_B T}\right)}$$

where 3N is the number of independent modes of the system.

f)

$$C_V = Nk_B \int_0^\infty d\omega \left(\frac{\hbar\omega}{2k_B T}\right)^2 \frac{DOS(\omega)}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)}$$

- The behaviour of C_V at small temperatures depends on the dimensionality through the density of states.

$$\omega = v\|q\| \Rightarrow DOS(\omega) = \text{const} \quad 1D$$

$$DOS(\omega) \propto \omega \quad 2D$$

$$DOS(\omega) \propto \omega^2 \quad 3D$$

$$\Rightarrow C_V = Nk_B \int_0^\infty d\omega \left(\frac{\hbar\omega}{2k_B T}\right)^2 \frac{\alpha\,\omega^{d-1}}{\sinh^2\left(\frac{\hbar\omega}{2k_B T}\right)} \propto T^d \int_0^\infty dx \frac{x^{d-1}}{\sinh^2\left(\frac{x}{2}\right)} \qquad \frac{\hbar\omega}{k_B T} = x$$

where α is a constant and depends on dimensionality

4.2

The calculation of the grancanonical partition function in the fermionic case is identical up to the point

a)

$$Z = \prod_\lambda \sum_{n_\lambda = 0,1} \left[e^{-\beta(\varepsilon_\lambda - \mu)}\right]^{n_\lambda} = \prod_\lambda \left(1 + e^{-\beta(\varepsilon_\lambda - \mu)}\right)$$

b)

$$\langle \hat{n}_\lambda \rangle = -\frac{1}{\beta}\frac{\partial}{\partial \varepsilon_\lambda} \ln Z = -\frac{1}{\beta}\frac{\partial}{\partial \varepsilon_\lambda} \sum_{\lambda} \ln\left(1 + e^{-\beta(\varepsilon_{\lambda'} - \mu)}\right).$$

$$= \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} + 1}$$

$$\boxed{n_{FD}(\varepsilon_\lambda) = \frac{1}{e^{\beta(\varepsilon_\lambda - \mu)} + 1}}$$

FERMI DIRAC DISTRIBUTION

c) See attached plots

d)

$$U = -\frac{\partial}{\partial \beta} \ln Z + \frac{\mu}{\beta}\frac{\partial}{\partial \mu} \ln Z = \sum_\lambda \frac{\varepsilon_\lambda}{e^{\beta(\varepsilon_\lambda - \mu)} + 1} = \sum_\lambda n_{FD}(\varepsilon_\lambda)\, \varepsilon_\lambda .$$

The chemical potential of a bosonic system.

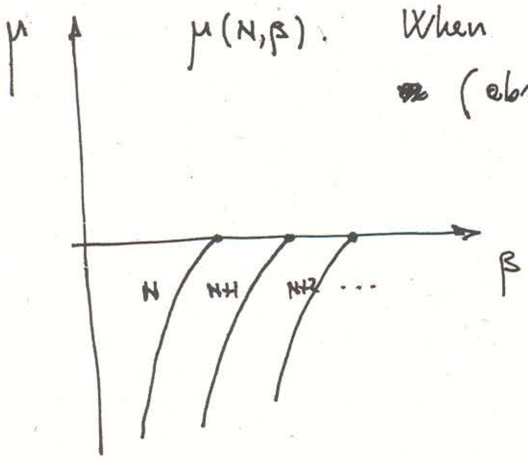
$$n_{BE}(E) = \frac{1}{e^{-\beta(E-\mu)} - 1}$$

Notice that in general the sum rule holds:

$$N = \int_0^\infty dE \; DOS(E)\, n_{BE}(E) \qquad (*)$$

where N is the total number of bosons. This sum rule is also used to calculate $\mu = \mu(T, N)$. If $\mu > \varepsilon_{min}$, where ε_{min} is the minimum energy of the system => the integral diverges. This is a reason for saying $\mu < \varepsilon_{min}$. For phonons with acoustic branches $\mu < 0$.

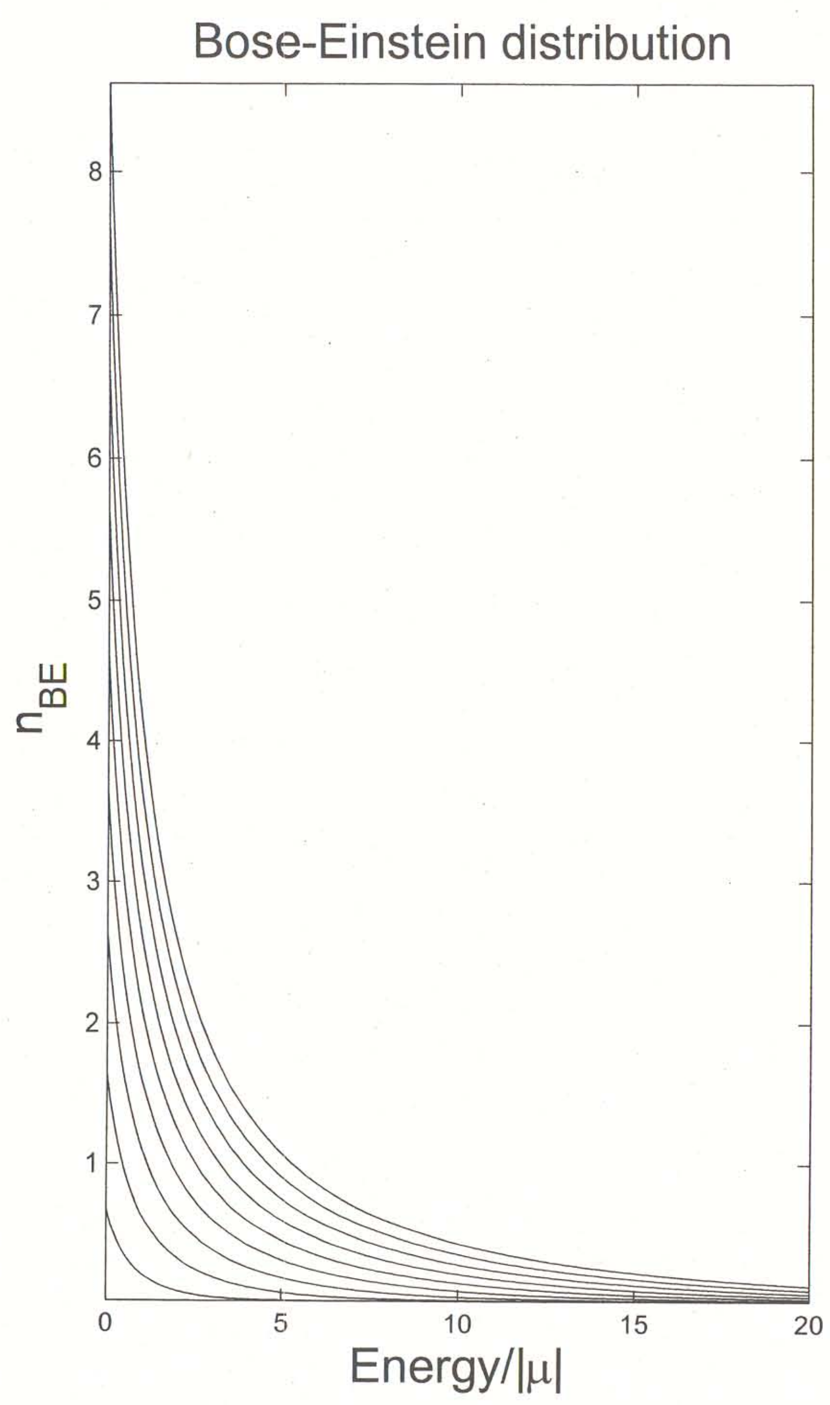
Finally a bit of BOSE-EINSTEIN CONDENSATION:

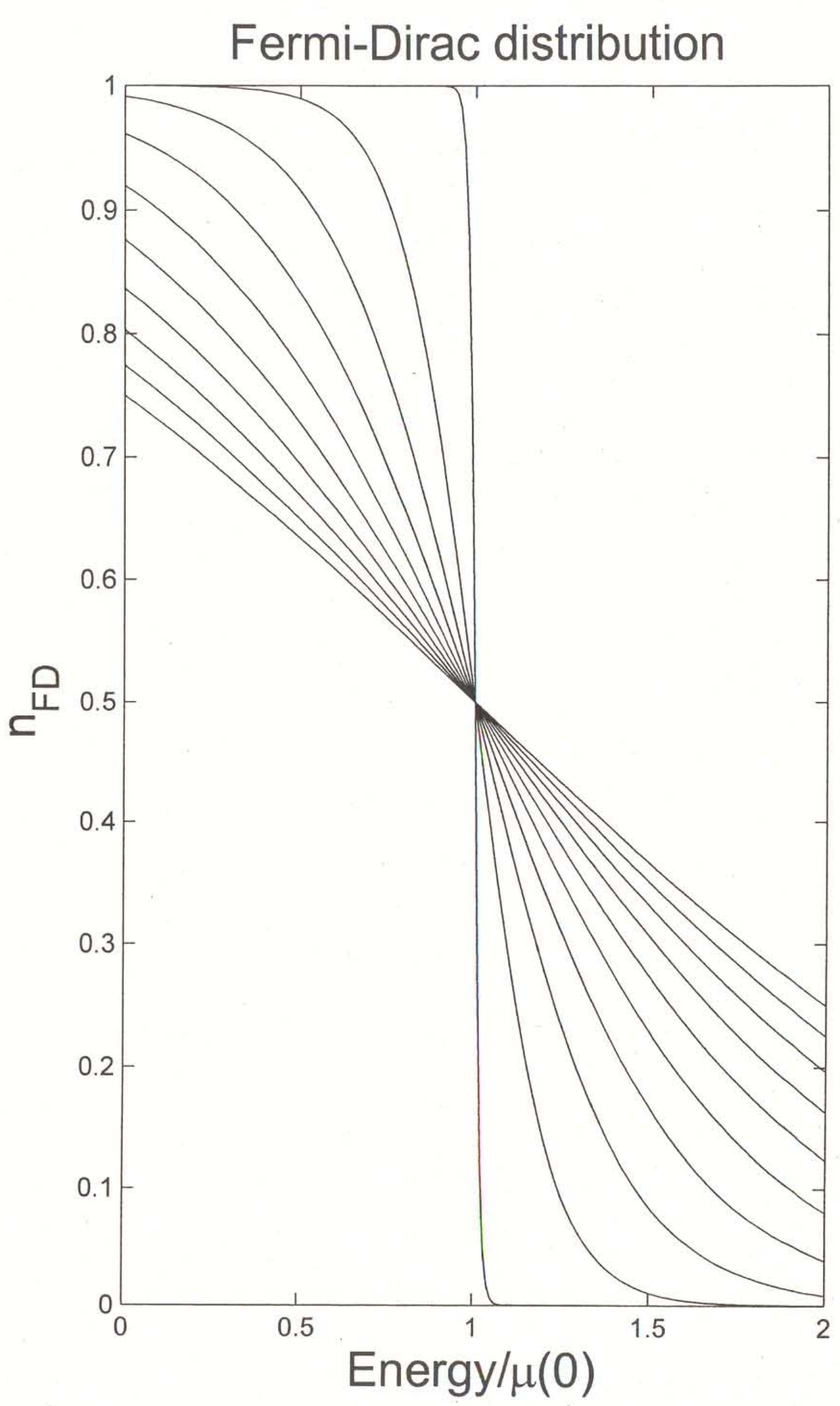


$\mu(N,\beta)$. When the solution of (*) for μ would give $\mu > \varepsilon_{min}$ (absurde) the physical solution exists:

$$N = N_0 + \int_{\varepsilon_{min}}^\infty dE \; DOS(E)\, n_{BE}(E)$$

finite fraction of bosons in the condensate.


Bose-Einstein distribution
n_{BE}
Energy/$|\mu|$
0
5
10
15
20
1
2
3
4
5
6
7
8


Fermi-Dirac distribution
n_{FD}
Energy/$\mu(0)$
0
0.5
1
1.5
2
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1