ADVANCED QUANTUM MECHANICS

https://github.com/Muatyz/review-sheet

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Contents

第一章　Homework

1.1　Homework 1

1.1.1　Hermitian operators

1. **Prove theorem 1: If A is Hermitian operator, then all its eigenvalues are real numbers, and the eigenvectors corresponding to different eigenvalues are orthogonal.**

2. **Prove theorem 2: If A is Hermitian operator, then it can be always diagonalized by unitary transformation.**

3. **Prove theorem 3: Two diagonalizable operators A and B can be simultaneously diagonalized if, and only if, $[A, B] = 0$.**

1.1.2 Matrix diagonalization and unitary transformation

1. **Diagonalizing a matrix L corresponds to finding a unitary transformation V such that $L = V\Lambda V^{\dagger}$, where Λ is a diagonal matrix whose diagonal elements are eigenvalues, V is an unitary matrix whose column vectors are the corresponding eigenstates. Find a unitary matrix V that can diagonalize the Pauli matrix $\sigma^{x}_{(z)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and find the eigenvalues of $\sigma^{x}_{(z)}$.**

2. **The three components of the spin angular momentum operator $\vec{S}$ for spin-$1/2$ are S^x, S^y, and S^z. If we use the S^z representation, their matrix representations are given by $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, where the three components of $\vec{\sigma}$ are the Pauli matrices σ^x, σ^y, and σ^z.**

   Now consider using the S^x representation. Please list the order of basis vectors you have chosen in the S^x representation, and calculate the matrix representations of the three components of the operator $\vec{S}$ in this representation.

1.2 Homework 2

1.2.1 Angular momentum for 4-dimensional space

Consider a 4-dimensional space with coordinates (x, y, z, w).

1. **Show that the operators $L_i = \epsilon_{ijk} x_j p_k$ and $K_i = w p_i - x_i p_w$ generate rotations in this space by showing that the transformations generated by these operators leave the four dimensional radius, defined by $R^2 = x^2 + y^2 + z^2 + w^2$, invariant.**

2. **Compute the commutators $[L_i, K_j]$ and $[K_i, K_j]$.**

1.2.2 Harmonic oscillator

1. **Find the energy eigenvalues E_n and the corresponding wave functions $\psi_n(x)$ for a one-dimensional quantum harmonic oscillator system.**

2. **Calculate $\langle m|x|n\rangle$, $\langle m|p|n\rangle$, $\langle m|x^2|n\rangle$, and $\langle m|p^2|n\rangle$.**

3. **Assume the quantum harmonic oscillator is in a thermal bath at temperature T; find the partition function Z and the average energy $\langle E\rangle$ of the system.**

4. **Prove that the inner product of coherent states is given by:**

$$\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta}$$

1.3 Homework 3

1.3.1 Schwinger boson representation

A two-dimensional quantum harmonic oscillator contains two decoupled free bosons, whose annihilation operators can be represented as a and b respectively. $a = \dfrac{1}{\sqrt{2}}(x + ip_x)$, $b = \dfrac{1}{\sqrt{2}}(y + ip_y)$. They satisfy the commutation relations $[a, a^\dagger] = [b, b^\dagger] = 1$ and $[a, b] = [a, b^\dagger] = 0$. This system has U(2) symmetry, which includes an SU(2) subgroup. Let's explore how to construct the SU(2) representation using bosonic operators. Define $S^x = \dfrac{1}{2}(a^\dagger b + b^\dagger a)$, $S^z = \dfrac{1}{2}(a^\dagger a - b^\dagger b)$.

1. **Express S^y in terms of a and b. [Hint: Make $\vec{S} \times \vec{S} = i\vec{S}$]**

2. **Prove that S^y is actually related to the angular momentum operator of the harmonic oscillator $L = xp_y - yp_x$, namely $S^y = \dfrac{L}{2}$.**

$\square$

3. **Define the following set of states, where $s = 0, 1/2, 1, \cdots$, and $m = -s, -s+1, \cdots, s-1, s$ (they are called the Schwinger boson representation),**

$$|s, m\rangle = \frac{(a^\dagger)^{s+m}}{\sqrt{(s+m)!}} \frac{(b^\dagger)^{s-m}}{\sqrt{(s-m)!}} |\Omega\rangle$$

where $|\Omega\rangle$ is the state annihilated by a and b, i.e., $a|\Omega\rangle = b|\Omega\rangle = 0$. Prove that the state $|s, m\rangle$ is indeed a simultaneous eigenstate of $\vec{S}^2 = (S^x)^2 + (S^y)^2 + (S^z)^2$ and S^z , with eigenvalues $s(s+1)$ and m respectively. [Hint: Use the particle number basis.]

□

1.3.2 1D tight-binding model

The Hamiltonian of a periodic tight-binding chain of length L is given by the following expression:

$$H_{\textbf{chain}} = -t \sum_{n=1}^{L} \left(\hat{a}_n^\dagger \hat{a}_{n+1} + \hat{a}_{n+1}^\dagger \hat{a} \right)$$

where t is the hopping matrix element between adjacent sites n and $n+1$, $\hat{a}_n^\dagger$ creates a fermion at site n, and the set of operators $\{a_n^\dagger, a_n; n = 1, \cdots, L\}$ satisfies the standard anticommutation relations:

$$\{a_n, a_{n'}^\dagger\} = \delta_{nn'}, \quad \{a_n, a_{n'}\} = 0, \quad \{a_n^\dagger, a_{n'}^\dagger\} = 0$$

We assume periodic boundary conditions, i.e., we consider $a_{L+n}^\dagger = a_n^\dagger$.The purpose of this problem is to prove that this Hamiltonian can be diagonalized by a linear transformation of the discrete Fourier transform form:

$$b_k^\dagger = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger$$

1. **Let's require that $b_k^\dagger$ remains invariant under any shift of the summation index $n \to n + n'$ ("translation invariance"). Prove that this implies that the index k is quantized and determine the set of allowed k values. How many independent $b_k^\dagger$ operators are there?**

2. **Verify that the set of b_k and $b_k^\dagger$ operators also satisfies the above standard anticommutation relations. That is:**

$$\{b_k, b_{k'}^\dagger\} = \delta_{kk'}, \quad \{b_k, b_{k'}\} = 0, \quad \{b_k^\dagger, b_{k'}^\dagger\} = 0$$

Hint: Use the identity $\sum_{m=1}^{L} e^{i\frac{2\pi}{L}m} = 0$.

3. **Prove that the inverse transformation of the above has the form:**

$$a_n^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{-ikn} b_k^\dagger$$

where the sum is over the set of allowed k values determined in (a).

4. **Show that $b_k^\dagger$ is indeed a creation operator of a single-particle eigenstate of H_{chain} by proving that its commutator with the Hamiltonian has the form $[H_{\text{chain}}, b_k^\dagger] = \varepsilon_k b_k^\dagger$. Give the explicit expression for the corresponding eigenvalue ε_k.**

1.4 Homework 4

1.4.1 Mean-field Solutions for Extended Hubbard Model

The Hamiltonian of the extended Hubbard model can be written as:

$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + \textbf{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j$$

where:

- $c_{i\sigma}^\dagger$ **and** $c_{i\sigma}$ **are the fermionic creation and annihilation operators for an eletron with spin** σ **at site** i**.**
- $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ **is the number operator for electrons with spin** σ **at site** i**.**
- $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$ **is the number operator for total electrons at site** i**.**
- $U > 0$ **is the strength of the on-site interaction between electrons.**
- $V > 0$ **is the strength of the interaction between electrons at neighboring sites.**
- $t > 0$ **is the hopping strength of the electrons.**

We consider the case of half-filling for two lattice sites ($\langle N\rangle = \langle n_{1\uparrow} + n_{1\downarrow} + n_{2\uparrow} + n_{2\downarrow}\rangle$). In the mean-field approximation, calculate the ground state energy E_{MF}. Please consider initial mean-field values with following four cases.

1. **Case 1: Paramagnetic(PM). Initial mean-field value $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$.**

2. **Case 2: Ferromagnetic(FM). Initial mean-field value $\langle n_{i\uparrow}\rangle = 1$ and $\langle n_{i\downarrow}\rangle = 0$.**

3. **Case 3: Anti-ferromagnetic(AFM). Initial mean-field value** $\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1-\alpha$ **and** $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \alpha$**.**

4. **Case 4: Charge density wave(CDW). Initial mean-field value** $\langle n_{1\uparrow}\rangle = \langle n_{1\downarrow}\rangle = 1-\alpha$ **and** $\langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \alpha$**.**

1.5 Homework 5

1.5.1 Quantum Rotor Model

The angular coordinate of a quatum rotor is $\theta \in [0, 2\pi)$, note that $\theta \pm 2\pi$ and θ are equivalent. The eigenstate of the operator $\hat{\theta}$ is represented by $|\theta\rangle$, and $\theta \pm 2\pi\rangle$ represents the same state as $|\theta\rangle$. Define the rotation operator for the quantum rotator as $\hat{R}(\alpha)$,

$$\hat{R}(\alpha) = \int_0^{2\pi} \mathrm{d}\theta |\theta - \alpha\rangle\langle\theta|$$

Thus $\hat{R}(\alpha)|\theta\rangle = |\theta - \alpha\rangle$, and $\hat{R}(2\pi)$ is the identity operator.

The rotation operator $\hat{R}(\alpha)$ is a unitary operator, its generator is the Hermitian operator $\hat{N}$, which is related to the angular momentum operator of the quantum rotator $\hat{L}$ by $\hat{L} = \hbar\hat{N}$, so $\hat{R}(\alpha) = e^{i\hat{N}\alpha}$, and in the $\hat{\theta}$ representation, we have $\hat{N} = -i\frac{\partial}{\partial\theta}$.

Consider a specific quantum rotor model, its Hamiltonian is

$$\hat{H} = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2 - g\cos 2\hat{\theta}$$

where $g\cos 2\hat{\theta}$ is a small external potential, which can be treated as a perturbation. Assuming $|N\rangle$ is the eigenstate of the operator $\hat{N}$ with eigenvalue N, i.e., $\hat{N}|N\rangle = N|N\rangle$. It can be calculated that $|N\rangle$ is expanded in terms of $|\theta\rangle$ as

$$|N\rangle = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle$$

1. **Use the fact that $\hat{R}(2\pi)$ is the identity operator to prove that N must be an integer.**

2. **Consider the unperturbed Hamiltonian $\hat{H}_0 = \frac{1}{2}\left(\frac{1}{2}\hat{N} - \frac{1}{2}\right)^2$, prove that $|N\rangle$ is also an eigenstate of $\hat{H}_0$, and find its eigenenergy, demonstrating that each energy level is doubly degenerate.**

3. **Using the basis set $\{|N\rangle\}$, write down the representation matrix for the perturbation term $\hat{V} = -g\cos 2\hat{\theta}$, and prove that the perturbation does not connect degenerate levels (i.e., if $|N\rangle$ and $|N'\rangle$ are degenerate, then $\langle N|\hat{V}|N'\rangle = 0$). Therefore, although the energy levels of $\hat{H}_0$ are degenerate, we can still use non-degenerate perturbation theory.**

4. **Calculate the perturbation correction to each energy level E_N up to second order in g, and prove that all degeneracies of the energy levels remain unlifted.**

第二章　2022秋高等量子力学期末考核

2.1　单项选择

1. 让大量热化的自旋通过 **Stern-Gerlach** 装置**SG** $\hat{z}$,测得 S_+^z 的概率是**?**

2. **Pauli** 矩阵 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, 那么 $\sigma^x\sigma^z$ 等于**?**

3. 混态可以用混态的密度矩阵来描述. 假设系统处于态 $|\phi_i\rangle$ 的概率为 p_i, 注意 $\sum_i p_i = 1$, 那么该系统的密度矩阵为 $\rho = \sum_i |\phi_i\rangle p_i \langle\phi_i|$, 那么 **Tr**$[\rho]$ 应满足**?**

4. 如果 ρ 是混态的密度矩阵, 那么 **Tr**$[\rho^2]$ 应满足**?**

5. 考虑系统哈密顿量 H 不显含时间, 时间演化算符为 $U(t,0) = e^{-iHt/\hbar}$. 在海森堡绘景中, 我们让算符承载时间演化, 海森堡绘景中的算符定义为 $A_H(t) = U^\dagger(t,0)AU(t,0)$, 其中 A 是薛定谔绘景中的算符, 如果 A 不显含时间, 那么 $\mathrm{d}A_H(t)/\mathrm{d}t$ 等于**?**

6. 电磁场中电荷为 q 的单粒子哈密顿量为 $H = \dfrac{(\vec{p} - q\vec{A})^2}{2m} + q\phi$, 那么薛定谔方程 $i\hbar\dfrac{\partial\psi}{\partial t} = H\psi$ 满足规范不变性: $\vec{A} \to \vec{A} - \nabla\Lambda$, $\phi \to \phi + \dfrac{\partial\Lambda}{\partial t}$, $\psi \to$**?**

7. 角动量的对易关系为 $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$**,** 升降算符定义为 $J_\pm = J_x \pm iJ_y$**,** 那么 $[J_+, J_-] =$**?**

8. 二维谐振子的哈密顿量为 $H = \hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right)$ 其第一激发态的简并度为**?**

9. 量子比特 A 和 B 构成双量子比特体系**,** 双量子比特态 $|\psi\rangle$ 中量子比特 A 的纠缠熵定义为 $S(A) = -\mathbf{Tr}[\rho_A \ln \rho_A]$**,** 其中 ρ_A 是约化密度矩阵**,** 由密度矩阵求迹掉量子比特 B 的自由度得到**.** 考虑自旋单态 $|\psi\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$**,** 计算可得量子比特 A 的纠缠熵为**?**

10. 假设哈密顿量 H 是厄密的, 其基态能量为 E_0, 给定某个态Ψ, 测得能量期望值为 $E[\Psi] = \dfrac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$, $E(\Psi)$ 和 E_0 的关系为?

2.2 多项选择

1. 与总角动量算符的平方 $\vec{J}^2$ 对易的算符在 $(J_x, J_y, J_z, J_+, J_-)$ 中有?

2. 在原子单位制下 $\hbar = c = 1$, 和能量同单位的量在 (距离, 动量, 时间, 质量, 角动量) 中有?

3. 宇称算符 $\mathbb{P}$ 连续作用两次为恒等变换, 这说明宇称算符 $\mathbb{P}$ 的本征值在 $(0, 1, -1, i, -i)$ 中有?

4. 如果算符 A 满足 $A^2 = A$, 那么算符 A 的本征值有 $(0, 1, -1, i, -i)$ 中有?

5. 玻色子产生和湮灭算符满足对易关系 $\left[b_\alpha^\dagger, b_\beta^\dagger\right] = [b_\alpha, b_\beta] = 0$, $\left[b_\alpha, b_\beta^\dagger\right] = \delta_{\alpha\beta}$, 那么和总粒子数算符 $N = \sum_\alpha b_\alpha^\dagger b_\alpha$ 对易的算符在 $(b_\alpha, b_\alpha^\dagger b_\alpha, b_\alpha^\dagger b_\beta, b_\alpha^\dagger b_\beta b_\mu, b_\alpha^\dagger b_\beta b_\mu^\dagger b_\nu)$ 中有?

2.3 简答题

1. 中心势场中的单粒子哈密顿量为 $H = \dfrac{\vec{p}^2}{2M} + V(r)$. 轨道角动量 $\vec{L} = \vec{r} \times \vec{p}$, 那么 $[\vec{L}, H] =?$

2. 考虑一阶近似, 当 $i \neq f$ 时, 跃迁概率为

$$P_{i\to f}(t) = \frac{1}{\hbar^2}\left|\int_0^t \mathrm{d}t' \langle f|V(t')|i\rangle e^{\mathrm{i}\omega_{fi}t'}\right|^2$$

其中 $\hbar\omega_{fi} = E_f - E_i$. 当微扰为

$$V(t) = \begin{cases} Ve^{-\mathrm{i}\omega t} & t > 0 \\ 0 & t < 0 \end{cases}$$

跃迁概率为?

3. *

4. 动量空间中自由粒子的 **Dirac** 方程可以写为

$$(E - \vec{\sigma}\cdot\vec{p})\,\chi_+(\vec{p}) = m\chi_-(\vec{p}), \quad (E + \vec{\sigma}\cdot\vec{p})\,\chi_-(\vec{p}) = m\chi_+(\vec{p})$$

当质量 $m = 0$时, 两个 **Weyl** 旋量之间没有耦合, 得到动量空间中的 **Weyl** 方程

$$(E - \vec{\sigma}\cdot\vec{p})\,\chi_+ = 0, \quad (E + \vec{\sigma}\cdot\vec{p})\,\chi_- = 0$$

定义螺旋度算符为 $\frac{1}{2}\hat{\vec{p}}\cdot\vec{\sigma}$, 其中 $\hat{\vec{p}} = \frac{\vec{p}}{|\vec{p}|}$, 那么可知 **Weyl** 旋量 $\chi_\pm$ 恰好是螺旋度算符的本征态, 本征值分别为?

5.

2.4 应用题

1. 矩阵对角化和表象变换

(a) 对角化矩阵 L 就是去找到幺正变换 V, 使得 $L = V\Lambda V^\dagger$, 其中 Λ 是一个对角矩阵, 它的对角元是本征值. V 是一个幺正矩阵, 它的列矢量是本征矢, 和 Λ 中的本征值一一对应. 找到一个能对角化 **Pauli** 矩阵 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ 的幺正矩阵 V, 并找到 σ^x 的本征值.

(b) 自旋 $1/2$ 的自旋角动量算符 $\vec{S}$ 的三个分量为S^x, S^y, S^z. 如果采用 S^z 表象, 它们的矩阵表示为 $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, 其中 $\vec{\sigma}$ 的三个分量为 **Pauli** 矩阵 σ^x, σ^y, σ^z. 现在考采用 S^x 表象, 请列出 S^x 表象中你约定的基矢顺序, 并求出在该表象下算符 $\vec{S}$ 的三个分量的矩阵表示.

2. 谐振子问题

一维谐振子的哈密顿量为

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

坐标算符 x 和动量算符 p 满足对易式 $[x, p] = i\hbar$. 对动量算符和坐标算符进行重新标度

$$p = P\sqrt{\hbar m\omega}, \quad x = Q\sqrt{\frac{\hbar}{m\omega}}$$

注意新的坐标算符 Q 和动量算符 P 是无量纲的, 哈密顿量重新写为

$$H = \frac{1}{2}\hbar\omega(P^2 + Q^2)$$

引入玻色子产生和湮灭算符, $a^\dagger$ 和 a.

$$a = \frac{1}{\sqrt{2}}\left(Q + iP\right), \quad a^\dagger = \frac{1}{\sqrt{2}}\left(Q - iP\right)$$

(a) 计算 $[Q, P]$, $[a, a^\dagger]$, $[a, a^\dagger a]$, $[a^\dagger, a^\dagger a]$;

(b) 将哈密顿量 H 用 a 和 $a^\dagger$ 表示. 并求出全部能级;

(c) 在能量表象中, 计算 a 和 $a^\dagger$ 的矩阵元.

3. 角动量耦合

两个大小相等, 属于不同自由度的角动量 $\vec{J}_1$ 和 $\vec{J}_2$ 耦合成总角动量 $\vec{J} = \vec{J}_1 + \vec{J}_2$, 设 $\vec{J}_1^2 = \vec{J}_2^2 = j(j+1)\hbar^2$, $J^2 = J(J+1)\hbar^2$, $J = 2j, 2j-1, \cdots, 1, 0$. 在总角动量量子数 $J = 0$ 的状态下, 求 $J_{1,z}$ 和 $J_{2,z}$ 的可能取值及相应概率.

4. 自旋-1 模型

考虑自旋-1 体系, 自旋算符为 $\vec{S}$, 考虑 $(\vec{S}^2, S^z)$ 表象, 基矢顺序为 $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$, 简记为 $|+1\rangle$, $|0\rangle$, $|-1\rangle$. 设 $\hbar = 1$.

(a) 写出 S^x 和 S^z 的矩阵表示.

(b) 考虑哈密顿量 $H(\lambda) = H_0 + \lambda V$, 其中 $H_0 = (S^z)^2, V = S^x + S^z$. 考虑为 λV 微扰, 利用微扰论计算微扰后的各能级和各能态, 其中能级微扰准确到二阶, 能态微扰准确到一阶.

5. 均匀电子气

考虑三维相互作用均匀电子气, 哈密顿量为 $H = H_0 + H_I$. 考虑系统体积为 $V = L^3$, 每个方向的系统尺寸为 L. 采用箱归一化, 所以 $\vec{k}$ 是离散的, $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$, n_x, n_y, n_z 为整数. 采用二次量子化的语言, 可给出哈密顿量在动量空间的形式. H_0 为单体部分:

$$H_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$$

其中 $\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$ 是自由电子的色散关系. 用 ε_F 表示费米能, k_F 表示费米波矢的大小.

H_I 为两体相互作用部分,

$$H_I = \frac{1}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \sum_{\sigma\sigma'} v(q) c^\dagger_{\vec{k}_1+\vec{q},\sigma} c^\dagger_{\vec{k}_2-\vec{q},\sigma'} c_{\vec{k}_2\sigma'} c_{\vec{k}_1\sigma}$$

$v(q)$ 是相互作用 $v(x)$ 的傅里叶变换形式, $q = |\vec{q}|$, $x = |\vec{x}|$,

$$v(q) = \frac{1}{V} \int v(x) e^{-i\vec{q}\cdot\vec{x}} \mathrm{d}^3\vec{x}$$

这里我们考虑短程势, 也就是说 $v(q = 0)$ 不发散.

自由电子气零温下处于电子填充到费米能 ε_F 的费米海态(**Fermi sea state**), 简记为 **FS**, 利用费米子产生算符作用到真空态上可以表示 **FS** 态为

$$|\mathbf{FS}\rangle = \prod_{k<k_F,\sigma} c^\dagger_{\vec{k}\sigma} |0\rangle$$

(a) 考虑零温下的自由电子气, 计算总粒子数 N 和粒子数密度 n, 计算总能量 $E^{(0)}$ 并把总能量密度 $E^{(0)}/V$ 表示成粒子数密度 n 的函数.

(b) 计算能量的一阶修正 $E^{(1)} = \langle \mathbf{FS}|H_I|\mathbf{FS}\rangle$.

(c) 利用 **Hatree Fock** 平均场近似, 并假设平均场参数是自旋对角的, 并且保持了自旋对称性, 以及平移对称性, 因此我们期待 $\left\langle c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}'\sigma'} \right\rangle = \left\langle c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}\sigma} \right\rangle \delta_{\vec{k},\vec{k}'} \delta_{\sigma,\sigma'}$, 以及 $\left\langle c_{\vec{k}\uparrow}^{\dagger} c_{\vec{k}\uparrow} \right\rangle = \left\langle c_{\vec{k}\downarrow}^{\dagger} c_{\vec{k}\downarrow} \right\rangle$. 计算系统总能量, 并与 $E^{(0)} + E^{(1)}$ 比较大小.

6. 量子转子模型

量子转子的角度坐标 $\theta \in [0, 2\pi)$, 注意 $\theta \pm 2\pi$ 和 θ 是等价的. 用 $|\theta\rangle$ 表现 $\hat{\theta}$ 算符的本征态, $|\theta \pm 2\pi\rangle$ 和 $|\theta\rangle$ 是相同的态. 定义量子转子的转动算符为 $\hat{R}(\alpha)$,

$$\hat{R}(\alpha) = \int_0^{2\pi} \mathrm{d}\theta |\theta - \alpha\rangle\langle\theta|$$

所以 $\hat{R}(\alpha)|\theta\rangle = |\theta - \alpha\rangle$, 并且 $\hat{R}(2\pi)$ 是单位算符.

转动算符 $\hat{R}(\alpha)$ 是一个幺正算符, 它的产生子为厄米算符 $\hat{N}$, 与量子转子的角动量算符 $\hat{L}$ 的关系为 $\hat{L} = \hbar\hat{N}$, 所以 $\hat{R}(\alpha) = e^{i\hat{N}\alpha}$, 在 $\hat{\theta}$ 表象下可求得 $\hat{N} = -i\frac{\partial}{\partial\theta}$.

考虑一个特定的量子转子模型, 它的哈密顿量为

$$H = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2 - g\cos\left(2\hat{\theta}\right)$$

其中 $g\cos\left(2\hat{\theta}\right)$ 是一个小的外势, 可以当成微扰处理. 假设 $|N\rangle$ 是算符 $\hat{N}$ 的本征态, 本征值为 N, 即 $\hat{N}|N\rangle = N|N\rangle$. 可计算出 $|N\rangle$ 用 $|\theta\rangle$ 展开为

$$|N\rangle = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} e^{iN\theta}|\theta\rangle$$

(a) 利用 $\hat{R}(2\pi)$ 是单位算符证明 N 必须是整数.

(b) 考虑无微扰时的哈密顿量 $H_0 = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2$, 证明 $|N\rangle$ 也是 H_0 的本征态, 并求出本征能量, 证明每个能级都是两重简并的.

(c) 采用 $\{|N\rangle\}$ 作为基组, 写出微扰项 $V = -g\cos\left(2\hat{\theta}\right)$ 的表示矩阵, 并证明微扰不会连接简并的能级(即如果 $|N\rangle$ 和 $|N'\rangle$ 简并, 那么 $\langle N|V|N'\rangle$). 因此尽管 H_0 的能级是简并的, 我们仍然可以使用非简并微扰论.

(d) 计算每个能级 E_N 的微扰修正到 g 的二阶, 并证明此时所有的能级简并仍然没有被解除.