

## Quantum Mechanics (I): Homework 6

### December 28, 2011

**Ex.1 10** Show that for the  $n$ th eigenstate  $|n\rangle$  of a simple harmonic oscillator, the following equality holds for any positive integer  $k$

$$\langle n | (m\omega \hat{x})^{2k} | n \rangle = \langle n | \hat{p}^{2k} | n \rangle.$$

**Ex.2** Consider a coherent state  $|\lambda, t\rangle$ .

(a) **5** The probabilities of finding  $|\lambda\rangle$  ( $= |\lambda, 0\rangle$ ) in  $|n\rangle$  is  $|\langle n|\lambda\rangle|^2$ , what kind of distribution is it?

(b) **5** What is the average number of *quanta* (i.e.,  $n$ ) in  $|\lambda\rangle$ ?

(c) **10** What is the standard deviation (i.e.,  $\Delta n$ ) of  $n$ ? Show that the so-called factorial cumulants  $\kappa_p \equiv \langle n(n-1)(n-2)\cdots(n-p+1)\rangle - \langle n\rangle^p$  vanish for any  $p$ .

(d) **10** Let  $\psi_\lambda(x, t) = \langle x | \lambda, t \rangle$ , find  $\psi_\lambda(x, t)$ .

(e) **15** Consider  $t = 0$ , let  $\lambda$  be real and  $\lambda \equiv \sqrt{2}s$ . Using the results of (d), show that

$$e^{-s^2+2ys} = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(y)$$

i.e.,  $\exp(-s^2 + 2ys)$  is the generating function of the Hermite polynomials  $H_n(y)$ .

(f) **15** Following the derivatin of the coherent state in the class, if we displace the average position and the momentum of the  $n$ th energy eigenstate by  $x_0$  and  $p_0$  at  $t = 0$ , find the wavefunction at  $t > 0$ . Verify that the average position moves exactly in the same way as that of the classical particle.

**Ex.3 10** Page 212, ex. 7.4.4.

**Ex.4 10** Page 212, ex. 7.4.5.

**Ex.5** Consider a particle of mass  $m$  subject to a one-dimensional potential of the following form:

$$V = \begin{cases} \frac{1}{2}kx^2 & \text{for } x > 0 \\ \infty & \text{for } x < 0 \end{cases}$$

(a) **5** What is the ground-state energy?

(b) **5** What is  $\langle x^2 \rangle$  for the ground state?

(c) **5** Find  $\langle \frac{1}{x^2} \rangle$  for the ground state.

(d) **7** Use the WKB approximation to estimate the ground-state energy and compare it with your answer of (a).

(e) **5** Find the orthonormal energy eigenfunctions for this potential.

**Ex.6 10** Page 258, ex. 10.1.3.

**Ex.7 10** Page 259, ex. 10.2.1.

**Ex.8 10** Consider two identical particles. Suppose that one is in the state  $\psi_a(x)$ , and the other is in the state  $\psi_b(x)$ . Let us denote the average of the square of their relative distance as  $\langle (x_1 - x_2)^2 \rangle_{\pm}$ , where  $+$  indicates the case when particles considered are bosons, and  $-$  indicates the case when particles considered are fermions. Show that averagely speaking, fermions have larger relative-distance; it differs from that of bosons by

$$\langle (x_1 - x_2)^2 \rangle_- - \langle (x_1 - x_2)^2 \rangle_+ = 4 \left( \int dx x \psi_a^*(x) \psi_b(x) \right)^2.$$

**Ex. 9 10** Page 278, ex.10.3.4.

**Ex. 10** Consider a particle characterized by the Hamiltonian

$$\hat{h} = \Delta [2|1\rangle\langle 1| - |2\rangle\langle 2| + 2(|1\rangle\langle 2| + |2\rangle\langle 1|)].$$

Here  $\Delta$  is a real number with the dimension of energy;  $|1\rangle$  and  $|2\rangle$  are normalized and are also orthogonal to each other. We shall assume that statistics of such particles is bosonic. Suppose that a system is composed of three such particles.

(a) **10** Find the matrix of Hamiltonian ( $\equiv \hat{H}$ ) for this system in the Fock space. Here the index conventions are: 1 for  $|3, 0\rangle$ , 2 for  $|2, 1\rangle$ , 3 for  $|1, 2\rangle$ , and 4 for  $|0, 3\rangle$ . We use  $|n, m\rangle$  to represent the state with  $n$  particles in the state  $|1\rangle$  and  $m$  particles in the state  $|2\rangle$ .

(b) **15** Let the creation and annihilation operators for  $|1\rangle$  and  $|2\rangle$  be  $a_1^\dagger, a_2^\dagger$  and  $a_1, a_2$ . We can define another set of creation and annihilation operators for  $|I\rangle$  and  $|II\rangle$  be  $a_I^\dagger, a_{II}^\dagger$  and  $a_I, a_{II}$ , where  $|I\rangle$  and  $|II\rangle$  are eigenkets of  $\hat{h}$  with

largest and smallest eigenvalues respectively. Show that the Hamiltonian  $\hat{H}$  is diagonalized in terms of  $a_{\text{I}}^\dagger$ ,  $a_{\text{II}}^\dagger$ ,  $a_{\text{I}}$ , and  $a_{\text{II}}$  if

$$\begin{aligned} a_{\text{I}} &= \frac{1}{\sqrt{5}}(2a_1 + a_2), \\ a_{\text{II}} &= \frac{1}{\sqrt{5}}(a_1 - 2a_2), \end{aligned}$$

and  $(a_{\text{I}}^\dagger, a_{\text{II}}^\dagger, a_{\text{I}}, a_{\text{II}})$  satisfy “standard” commutation relations such as  $[a_{\text{I}}, a_{\text{II}}] = 0$  and  $[a_{\text{I}}, a_{\text{I}}^\dagger] = 1$ .

**Ex. 11 Crystal momentum versus momentum** As we learned in the class, if the Hamiltonian of a system  $\hat{H}(x)$  is invariant under infinitesimal translations  $\varepsilon$ , i.e.,  $\hat{H}(x + \varepsilon) = \hat{H}(x)$ , the momentum  $p$  of this system is conserved. In particular, the wavefunction  $\psi(x)$  is  $\exp(ipx/\hbar)$  up to a normalization constant. Thus,

$$\psi(x + a) = \exp(ika)\psi(x)$$

with  $k \equiv p/\hbar$  being the wavevector. The crystal momentum is resulted from considering a system that is translationally invariant only for  $\varepsilon = na$ , where  $a$  is a fixed constant and  $n$  is an integer. That is, when the system considered is periodic, the relevant quantity is the crystal momentum. A typical example is a system with a periodic potential  $V(x) = V_0 \sin(2\pi x/a)$ .

(a) **5** Show that in this case even though the energy eigenfunction is no longer a plane wave, the above equation is still correct with  $k$  being some constant not proportional to the real momentum. This is known as the *Bloch theorem*, and  $\hbar k$  is known as the crystal momentum.

(b) **5** From (a), prove the alternating form of the Bloch theorem, i.e., the wavefunction can be rewritten as

$$\psi(x) = \exp(ikx)u(x),$$

where  $u(x + a) = u(x)$  is some periodic function of period  $a$ . Wavefunctions of this kind are known as the Bloch functions.

(c) **5** Show that the conserved quantity is  $\exp(ika)$ , not  $k$ . This also reflects the fact that  $k$  is not uniquely defined, any combinations  $k + 2\pi m/a$  ( $m$  is some integer) give the same factor  $\exp(ika)$ . In particular, we allow the change  $k \rightarrow k + 2\pi m/a$  during the course of the time. This is known as the Umklapp process. See any textbooks on solid state for more details.

(d) **10** We now apply the above theorem to investigate the problem when a particle of mass  $m$  is in the one-dimensional potential

$$V(x) = -A \sum_{n=-\infty}^{n=\infty} \delta(x - na),$$

where  $A$  is a positive constant,  $n$  are integers and  $a$  is positive. Find the relation between the energy  $E$  and the crystal momentum  $k$  of the particle. Demonstrate that the energy spectrum consists of bands separated by forbidden gaps.

**Ex.12 Discrete Fourier Transformation and Phonons**

(a) **10** Consider a periodic function  $f(x)$  in  $0 \leq x < L$  with  $f(x + L) = f(x)$ . According to the Fourier expansion, one can expand

$$f(x) = \frac{1}{\sqrt{L}} \sum_{n=-\infty}^{\infty} a_n e^{i\frac{2n\pi}{L}x},$$

where we introduce the factor  $1/\sqrt{L}$  simply to make later forms more symmetric. By using

$$\int_0^L dx e^{i\frac{2m\pi}{L}x} e^{-i\frac{2n\pi}{L}x} = L\delta_{n,m}, \quad (1)$$

one can express  $a_n$  in terms of an integration over  $f(x)$ . Now suppose that  $x$  only resides on discrete points,  $x = ja$ ,  $j = 0, 1, 2, \dots, N - 1$  with  $a = \frac{L}{N}$ . If we replace all integrals by summation with the understanding that  $dx = a$  is small, show that one obtains the discrete Fourier transformation as follows

$$\begin{aligned} f_j &= \frac{1}{\sqrt{N}} \sum_k f_k e^{ik(ja)} \\ f_k &= \frac{1}{\sqrt{N}} \sum_j f_j e^{-ik(ja)}. \end{aligned}$$

What are the relations between  $k$  and  $n$  &  $f_k$  and  $a_n$ ? Find the discrete form of Eq.(1).

(b) Consider a system of  $N$  particles with classically equilibrium-positions being at  $x = ja$ ,  $j = 0, 1, 2, \dots, N - 1$ . Suppose that the mass of each particle is  $m$  and nearest-neighbouring particles are connected by springs with spring constant  $k$ . Therefore, the Hamiltonian of the system is

$$H = \frac{1}{2m} \sum_n p_n^2 + \frac{1}{2} m \omega_0^2 \sum_j (x_n - x_{n+1})^2,$$

where  $p_n$  and  $x_n$  are momentum and position operators of the  $n$ th particle. Using the discrete Fourier Transformation, express  $H$  in terms of the Fourier transformed momentum and position operators  $p_k$  and  $x_k$  (**10**). By appropriately defining creation and annihilation operators  $a_k$  and  $a_k^\dagger$ , show that  $H$  can be written in the form  $H = \sum_k \hbar \omega_k (a_k^\dagger a_k + 1/2)$  and find  $\omega_k$  ((a) **10**).

(c) **Bonus (0.5)** Assuming that  $N \gg 1$ , find the ground state wavefunction  $\Psi(x_0, x_1, x_2, \dots, x_{N-1})$  up to a normalization factor.

**Ex.13** Tensor product and exact diagonalization

(a) **8** Consider two two-level systems. Let the associated two levels are denoted by  $|1\rangle$  and  $|2\rangle$ , which are represented by

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

In this representation, each of the system is characterized by three observables denoted by  $\sigma_x^k$ ,  $\sigma_y^k$  and  $\sigma_z^k$ , which are given by

$$\sigma_x^k = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y^k = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z^k = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Here  $k$  is an index for the system so that  $k = 1$  or  $2$ . Suppose that two systems are governed by the Hamiltonian  $H = \sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2 + \sigma_z^1 \sigma_z^2$ . If we denote  $|1\rangle \otimes |1\rangle$ ,  $|1\rangle \otimes |2\rangle$ ,  $|2\rangle \otimes |1\rangle$ , and  $|2\rangle \otimes |2\rangle$  by  $(1, 0, 0, 0)^T$ ,  $(0, 1, 0, 0)^T$ ,  $(0, 0, 1, 0)^T$ , and  $(0, 0, 0, 1)^T$  respectively, find the matrix representation of  $H$ .

(b) **7** If we generalize (a) to three two-level systems with  $H = \vec{\sigma}^1 \cdot \vec{\sigma}^2 + \vec{\sigma}^2 \cdot \vec{\sigma}^3$ , where  $\vec{\sigma}^k = (\sigma_x^k, \sigma_y^k, \sigma_z^k)$ , find the matrix representation of  $H$ .

(c) **Bonus (1)** If we generalize (a) to  $N$  two-level systems with  $H = \sum_{n=1}^{n=N-1} \vec{\sigma}^n \cdot \vec{\sigma}^{n+1}$ ,  $H$  describes  $N$  interacting spins. Find numerical values of three lowest eigenvalues of  $H$  for  $N = 10$  (You may use any of your favorite software to write a program for solving this problem. The program must be handed in together with your solutions.)

**Bonus problem (+1)** How to prepare a coherent state?

In this problem, I am going to show you how to prepare a coherent state theoretically. First, consider a charge harmonic oscillator with mass  $m$  and charge  $q$  in a uniform electric field  $E(t)$ . The Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = (H_0 + H_1) |\psi(t)\rangle,$$

where  $H_0 = \hbar\omega(a^\dagger a + 1/2)$ . Verify that

$$H_1 = -q\sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)E(t).$$

(a) If we perform the transformation (i.e., use the so-called interaction picture)  $|\psi(t)\rangle_I = e^{iH_0 t/\hbar} |\psi(t)\rangle$ , show that the evolution operator for  $|\psi(t)\rangle_I$  is

$$U_I(t, 0) = \exp[i\phi(t)] \exp\left\{\int_0^t dt' [\alpha(t')a^\dagger - \alpha^*(t')a]\right\},$$

where

$$\phi(t) = \frac{q^2}{2m\hbar\omega} \int_0^t dt_1 \int_0^{t_1} dt_2 E(t_1)E(t_2) \sin \hbar\omega(t_1 - t_2),$$

and  $\alpha(t) = i\sqrt{1/2m\hbar\omega}E(t) \exp(i\hbar\omega t)$ .

(b) Show that the above result implies that if initially the system is in the ground state (at  $t = 0$ ), at time  $t$

$$|\psi(t)\rangle = \exp(-i\omega t/2) \exp[i\phi(t)] |\lambda(t)\rangle,$$

where  $\lambda(t) = e^{-i\omega t} \int_0^t dt' \alpha(t')$ . In other words, the particle evolves into a coherent state. By choosing  $E(t)$  appropriately, one can engineer the state at  $t$  into any desired coherent state.

(+1) (a) Use the coherent state to prove the Mehler summation formula

$$\begin{aligned} & \frac{1}{\sqrt{1-t^2}} \exp\left\{-\frac{1}{2(1-t^2)} [(x^2 + y^2)(1+t^2) - 4xyt]\right\} \\ &= \exp(-x^2/2 - y^2/2) \sum_{n=1}^{\infty} \frac{t^n}{2^n n!} H_n(x) H_n(y) \end{aligned}$$

(b) Exercise 21.1.21