Problem set 4, due on November 17, **before** the beginning of the lecture

1 Diffraction from a three-dimensional lattice (14 points)

Consider a three-dimensional lattice with primitive vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$, where $a_1 = 0.5$ nm, $a_2 = 1$ nm and $a_3 = 1.5$ nm, and the angle between $\mathbf{a}_1$ and $\mathbf{a}_2$ is 120°, while the other two angles are 90°.

a) Determine the distance between nearest planes of the family of lattice planes with the Miller indices (3, 2, 1). Hint: Recapitulate the definition of the Miller indices in the lecture and the correspondence between a family of lattice planes and a particular reciprocal lattice vector...

b) When performing a Bragg-scattering experiment using Cu-$K\alpha$ radiation with a wavelength of $\lambda = 0.154$ nm, what is the smallest scattering angle 2θ under which Bragg scattering from this family of lattice planes will be observed (i.e. first order scattering, n = 1 in the Bragg formula)?

2 Harmonic quantum oscillator (no points, is just intended for those interested as a supplement to the prereading due on this Thursday.)

One of the few exactly solvable problems in quantum mechanics is the harmonic oscillator. In analogy to the classical problem, in one dimension it is defined by the Hamiltonian

$$H = \frac{1}{2m}P^2 + \frac{1}{2}m\omega^2 Q^2, \tag{1}$$

where P and Q are the momentum and position operators, respectively, m is the particle mass and $\omega = \sqrt{K/m}$, K corresponding to the spring constant. Although quite simple, it is of paramount importance: There are many processes in physics which – to a good approximation – can be treated as harmonic. Apparently, the quantum oscillator model is a good starting point for the description of explicitly mechanical (quantization of vibrational modes in solids, "phonons") systems. As it turns out, also seemingly unrelated phenomena, such as the quantization of the radiation field ("photons"), can be modeled based on this formalism. In this exercise, we will discuss the basic features of the harmonic quantum oscillator to support the results we used in the lecture, like the "ladder" structure of the energy levels $E = (1/2+n)\hbar\omega(\mathbf{k})$ for the vibrational modes associated with $\mathbf{k}$ in a crystalline solid.

a) We introduce the new operators

$$\hat{Q} = \sqrt{\frac{m\omega}{\hbar}}Q, \quad \hat{P} = \frac{1}{\sqrt{m\hbar\omega}}P \tag{2}$$

The operators P and Q have the dimensions kg m/s and m, respectively. Show that $\hat{P}$ and $\hat{Q}$ are dimensionless and rewrite the Hamiltonian in the form $H = \hbar\omega\hat{H}$, where $\hat{H}$ depends on $\hat{Q}$ and $\hat{P}$.

An important concept for operators in quantum mechanics is related to the question whether it matters in which order two distinct operators A and B are applied on a wave function: If $A(B|\psi\rangle) = B(A|\psi\rangle)$, they are said to "commute", and the "commutator" $[A, B] = AB - BA$ is zero. This concept is closely related to Heisenberg's uncertainty principle: If two operators do *not* commute, then the physical quantities they represent cannot be measured simultaneously with arbitrary precision. The best-known example is $\Delta Q \cdot \Delta P \geq \hbar/2$.

Calculate $[Q, P]$ in one dimension in the position-space representation, in which $Q = x$ and $P = (\hbar/i)d/dx$. Hint: What is $[Q, P]\psi(x)$ for an arbitrary wave function $\psi(x)$? Do Q and P thus commute?

Calculate $[\hat{Q}, \hat{P}]$.

b) It is convenient to introduce the operators a, $a^\dagger$ and N:

$$a = \frac{1}{\sqrt{2}}(\hat{Q} + i\hat{P}), \quad a^\dagger = \frac{1}{\sqrt{2}}(\hat{Q} - i\hat{P}) \tag{3}$$

Calculate the commutator $[a, a^\dagger]$.

While $\hat{Q}$ and $\hat{P}$ are hermitian[1], this is not correct for $a^\dagger$ and a: $a^\dagger \neq a$. It follows, that a and $a^\dagger$ are no physical observables, i.e. they do not represent physically measurable quantities. Show that on the other hand the occupation number operator $N = a^\dagger a$ *is* hermitian. It is indeed an observable and represents a physically measurable quantity, as will be seen in c). Hint: Use the generally valid relation: $(AB)^\dagger = B^\dagger A^\dagger$.

Rewrite $\hat{H}$ in terms of $a^\dagger$, a and constants only. Rewrite $\hat{H}$ in terms of N and constants only.

c) In quantum mechanics, the eigenvectors of an observable form a basis of the Hilbert space of all possible wave functions, and the corresponding eigenvalues are real. With the results from b), show that the spectrum of the Hamiltonian H, i.e. the set of all possible eigenvalues, can be written in terms of the eigenvalues n of N: $E_n = \hbar\omega(n + \frac{1}{2})$, where $N|n\rangle = n|n\rangle$ and n is the eigenvalue corresponding to an eigenvector $|n\rangle$. It can be shown that

$$n \geq 0,\ a|0\rangle = 0,\ Na|n\rangle = (n-1)a|n\rangle \ \text{ if } n > 0 \ \text{ and } \ Na^\dagger|n\rangle = (n+1)a^\dagger|n\rangle \tag{4}$$

where $|0\rangle$ is the ground state and $|n\rangle$ is the n-th excited state. (You can prove the relations (4) as an optional exercise for 2 points). Why are therefore a and $a^\dagger$ called lowering and raising operator, respectively, or generally ladder operators? Show that the eigenvalues of N are $n = 0, 1, 2\ldots$ Hint: The assumption of an non-integer n leads to a contradiction with (4). Apply the ladder operators and draw a sketch of the “ladder”.

Which physical quantity does therefore the hermitian operator N represent?

d) Now the eigenvectors can be obtained from $|0\rangle$ by the successive application of $a^\dagger$:

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \tag{5}$$

Apart from a phase factor, in real-space representation $|0\rangle$ can be written as:

$$\langle x|0\rangle = \phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) \tag{6}$$

Use (5) to calculate ϕ_1 and ϕ_2. (Hint: Exploit the real-space representation of the momentum and position operators to obtain the real-space representation of $a^\dagger$.) Sketch ϕ_0, ϕ_1, ϕ_2 and $|\phi_0|^2$, $|\phi_1|^2$, $|\phi_2|^2$. Without further calculation, the expectation values $\langle Q\rangle$ and $\langle P\rangle$ are immediately evident. Is this in analogy to the classical harmonic oscillator? In other words, compare $\langle Q\rangle$ and $\langle P\rangle$ with the time-averaged position and momentum of a classical oscillator whose equilibrium position is at the origin.

Instead of comparing the averaged position, one can also have a look at the detailed probability *distribution* of finding the particle at a given x in the quantum-mechanical and classical case. Is there a difference between the QM and the classical case (no detailed calculation is required – a sketch and clever reasoning is enough).

[1] The operation $A^\dagger$ is called hermitian conjugation – it is the generalization of the complex conjugation of complex numbers to operators. In general, the hermitian conjugate $A^\dagger$ does not need to be equal to the original operator A. If it does, the operator is called a hermitian operator. You can, for instance, read the Wikipedia article `http://en.wikipedia.org/wiki/Bra-ket_notation` to gain further insight.