NTNU – Trondheim
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Department of Physics

Examination paper for

TFY4250/FY2045 Quantum Mechanics 1

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Permitted examination support material:
C: Basic calculators, Rottmann formula collection

Other information: ---

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ENGLISH VERSION:

1) The raising and lowering operators of the one-dimensional harmonic oscillator are defined by

$$a_{\pm} = \frac{1}{\sqrt{2}}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x \mp i\,\frac{p_x}{(m\hbar\omega)^{1/2}}\right].$$

a) Express x by a linear combination of the raising and lowering operator.

b) Evaluate the expectation value of x^4 for the ground state $|0>$, using the bra-ket notation, and the properties of the raising and lowering operators, which include

$$a_+ \,|n> = \,(n+1)^{\frac{1}{2}}\,|n+1>,$$

$$a_- \,|n> = \,\sqrt{n}\,|n-1>.$$

2) Let us assume that the spin state of an electron is in the spin-up eigenstate relative to the z-axis.

a) Explain in words your answers to the following questions:

i) If we measure the spin relative to the x-axis, what is the probability of finding the electron in the spin-up eigenstate (relative to the x-axis)?

ii) What is the corresponding expectation value of the spin (relative to the x-axis)?

iii) After measuring the spin relative to the x-axis, we measure the spin again relative to the z-axis. What is the probability of finding the electron now in the spin-up state relative to the z-axis?

b) Determine the answers to i) and iii) by computation. Keep it brief!

Hint: Use the corresponding, normalized eigenvectors of

$$\boldsymbol{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \boldsymbol{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

3) For an ideal gas of identical bosons, we found the following constraint that relates the amount of particles, the volume and the temperature:

$$N = \frac{V}{2\pi^2}\int_0^{\infty} \frac{k^2}{e^{[(\hbar^2 k^2/2m)-\mu]/k_B T}-1}\,dk.$$

As we lower the temperature, Bose condensation occurs when the chemical potential $\mu(T)$ hits zero and the above integral no longer describes the physical situation correctly.

a) Evaluate the integral at $\mu = 0$ and obtain the formula for the critical temperature T_c at which this happens.

b) How does T_c scale with the particle density?

Hint:

$$\int_0^{\infty} \frac{x^{s-1}}{e^x - 1}\,dx = \Gamma(s)\zeta(s)$$

Here, $\Gamma(s)$ is the gamma function and $\zeta(s)$ the Riemann zeta function, whose values are both $O(1)$ in this problem.

4) A particle moves within the potential

$$V(x) = \begin{cases} \frac{1}{2} m\omega^2 x^2 \;, & x > 0, \\ \infty \;, & x \leq 0. \end{cases}$$

a) Verify (without calculations!) that the exact ground state energy is $E_0 = \frac{3}{2}\hbar\omega$.

b) Use the variational method and the trial function

$$\varphi(x) = \begin{cases} cxe^{-\alpha x} & , \quad x > 0, \\ 0 & , \quad x \leq 0. \end{cases}$$

to estimate the ground state energy. How good is the estimate?

5) Derive the wave-function approximation of the WKB method by use of a power series. To do so, follow these steps:

i) Assume that the wave function can be written as

$$\psi(x) = A\, exp\left[\frac{i}{\hbar} S(x)\right]$$

where $S(x)$ is generally a complex function.

ii) Substitute this expression into the time-independent Schroedinger equation. Subsequently, eliminate the exponential function. You should find a nonlinear differential equation.

iii) Write $S(x)$ as a power series, according to

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2} S_2(x) + \cdots$$

Substitute this power series into the differential equation in ii), and write down the resulting differential equations at the zeroth order and at the first order (in $\hbar$)

iv) Show that

$$S_0(x) = \pm \int^x p(x')dx'$$

$$S_1(x) = \frac{i}{2} \ln p(x)$$

are the solutions of these zeroth and first-order differential equations, where we define $p(x) = \{2m[E - V(x)]\}^{1/2}$.

With this in mind, what is the approximate wave function of $\psi(x)$?

6) Let us derive the Numerov algorithm for the numerical solution of the one-dimensional, time-independent Schroedinger equation, which we rewrite as

$$\psi(x)'' + k(x)\psi(x) = 0 \tag{1}$$

with $k(x) = 2m[E - V(x)]/\hbar^2$. Given a discretization with step-size Δx, we use a Taylor expansion around ψ_n (with $\psi_n = \psi(x_n)$ and $x_n = x_0 + n \cdot \Delta x$) to approximate

$$\psi_{n+1} = \psi_n + \Delta x\, \psi_n' + \frac{\Delta x^2}{2} \psi_n'' + \frac{\Delta x^3}{6} \psi_n^{(3)} + \frac{\Delta x^4}{24} \psi_n^{(4)} + \frac{\Delta x^5}{120} \psi_n^{(5)}.$$

i) What is the corresponding approximation for ψ_{n-1}, using again a Taylor expansion around ψ_n?

ii) Add ψ_{n+1} and ψ_{n-1}. The derivatives of the resulting expression should only include second and fourth orders.

iii) Approximate the fourth-order derivative by

$$\psi_n^{(4)} = \frac{\psi_{n+1}'' + \psi_{n-1}'' - 2\psi_n''}{\Delta x^2}$$

and <u>then</u> replace all second derivatives by use of equation (1) above, where we define $k_n = k(x_n)$.

What is the resulting recursive equation for ψ_{n+1} in terms of ψ_n and ψ_{n-1}?