PHY662, Spring 2004
Outline for Tues. Feb. 10, 2004
MRI wrapup, C-G review

10th February 2004

1 Miscellaneous

1. Hand out homework #5.
2. Exam on Thursday. Hand out cover page. Possibility of a review session?
3. Mention variational method.
4. Today: go over MRI notes, review homework #4.

2 Variational method

In most cases, one cannot diagonalize the Hamiltonian exactly to find ground states, analytically. You then have recourse to at least 3 methods:

- Perturbation theory - solve an "easy" problem, then modify it slightly to make it into the real problem. Expand your answer in powers of the modification.
- Nonperturbative approximations. These include the variational method and allow for large changes to the eigenstates/values, but are often less "controlled".
- Numerical methods: solve as realistic a problem as possible, trying to be clever to reduce numerical errors.

The variational method for finding the ground state is easy to state:

> Choose a class of trial wave functions that may have one or more parameters: $\psi(x, \alpha, \beta, \gamma, \ldots)$, where x is the coordinate of the wave function and $\alpha, \beta, \gamma, \ldots$ are parameters that describe the family of trial wave functions. For best results, this wave function should reflect symmetries of

the problem and a good guess as to what a plausible ground state should look like. Then compute $\langle H \rangle$ as a function of the parameters and choose the values for the parameters that minimize $\langle H \rangle$. This gives an estimated ground-state wave function and ground-state energy.

3 Gaussian integrals

In the variational method and many, many other places in physics, one needs facility with Gaussian integrals. You will need such integrals for the homework due on Tuesday. In this homework, you will calculate the expectation value of the Hamiltonian for a Gaussian function. You will then vary the width of the Gaussian and find the width where $\langle H \rangle$ is minimized - this gives an estimate for the ground state and its energy. You have seen these integrals before, of course, this is just a reminder of the results and how to compute them. They are so very important that they bear repetition.

3.1 The simple Gaussian

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\pi/a}\,.$$

This can be shown by a trick where you square the integral and convert to polar coordinates. Let $N = \int_{-\infty}^{\infty} e^{-x^2}$. Then

$$\begin{aligned} N^2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\, e^{-x^2} e^{-y^2} \\ &= \int_0^{\infty}\int_0^{2\pi} rdrd\theta\, e^{-r^2}\, r \qquad [r^2 = x^2 + y^2] \\ &= 2\pi \int_0^{\infty} e^{-u}\, du/2 \qquad [u = r^2] \\ &= \pi\,. \end{aligned}$$

A change of variables $x \to x\sqrt{a}$ then gives the stated result.

3.2 Integrating the square

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2} = \frac{\pi}{2} a^{-3/2}\,.$$

This follows from simply taking the derivative with respect to a of the first result (on both sides of the equation and then multiplying through by -1).

3.3 Rewriting the results

Often, the exponential is not of the form $-ax^2$, but $\frac{x^2}{2\sigma^2}$, for a normalized Gaussian of rms width σ (variance σ^2), using $a = (2\sigma^2)^{-1}$:

$$\int_{-\infty}^{\infty} dx \, \frac{e^{-\frac{x^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}} = 1$$

and

$$\int_{-\infty}^{\infty} dx \, x^2 \frac{e^{-\frac{x^2}{2\sigma^2}}}{\sqrt{2\pi\sigma^2}} = \sigma^2 \, .$$