Homework #3 — Phys623 — Spring 1999
Deadline: 5 p.m., Wednesday, February 24, 1999.
Turn in homework in the class or put in the box on the door of Phys 2314 by 5 p.m.

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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of Schwabl.
Equation numbers without period, like (5), refer to the equations of this homework.

The Variational Principle (Chapter 11.2)

Using the variational principle, one finds the energy and the wave function of the ground state by minimizing the following expression (see Eq. (11.16)):

$$E(\mu) = \frac{\langle\psi_\mu|\hat{H}|\psi_\mu\rangle}{\langle\psi_\mu|\psi_\mu\rangle} = \frac{\int dx\, [-\frac{\hbar^2}{2m}\psi_\mu^*(x)\psi_\mu''(x) + V(x)|\psi_\mu(x)|^2]}{\int dx\, \psi_\mu^*(x)\psi_\mu(x)}, \tag{1}$$

where the primes denote derivatives in x. Integrating the first term in denominator by parts, Eq. (1) can be equivalently written as (show this!)

$$E(\mu) = \frac{\int dx\, [\frac{\hbar^2}{2m}|\psi_\mu'(x)|^2 + V(x)|\psi_\mu(x)|^2]}{\int dx\, \psi_\mu^*(x)\psi_\mu(x)}. \tag{2}$$

I strongly recommend you to use form (2), rather than form (1). In form (2) you need less derivatives to take, and the kinetic energy term is manifestly positive. You could use Mathematica or a similar program to take the integrals and, perhaps, even to minimize $E(\mu)$.

1. *Adapted from Qualifier, August 1990 and 1980, II-1.*

   Heavy quark (q) and its antiquark ($\bar{\text{q}}$) interact by linearly rising potential $U(r) = \sigma r$, where r is the distance between the particles, and form a bound state called quarkonium.

   (a) [**5 points**] Using the variational method, find (approximately) the energy and the wave function of the ground state.

   (b) [**5 points**] By definition, the Airy function $\mathrm{Ai}(x)$ satisfies the equation

   $$[d^2/dx^2 - x]\mathrm{Ai}(x) = 0 \tag{3}$$

   and vanishes when $x \to +\infty$. It oscillates when $x < 0$ and vanishes at a sequence of points x_n called the zeros of the Airy function:

   $$\mathrm{Ai}(x_n) = 0, \quad x_1 = -2.338, \quad x_2 = -4.088, \quad x_3 = -5.521, \quad \ldots \tag{4}$$

   Express the energy levels of quarkonium in terms of the zeros x_n of the Airy function. Compare the exact ground-state energy with the value found by the variational method in Part 1a.

   (c) [**3 points**] Using the WKB method, find approximate expressions for the Airy function in the limit $|x| \gg 1$ and for the energy levels E_n of quarkonium in the limit $n \gg 1$.

2. Consider a one-dimensional potential well of a given shape $U(x)$ with the characteristic depth U_0 and width a which obey the following inequality:[1)]

   $$\hbar^2/ma^2 \gg U_0, \tag{5}$$

   where m is the mass of a quantum particle moving in this potential. (Such a well is called *shallow*.)

[1)] The presence of the parameters U_0 and a does *not* imply that the shape of the potential well is rectangular. The word "characteristic" indicates that these are the parameters that characterize the overall size of the potential $U(x)$, which may have an arbitrary shape.

(a) [**5 points**] Using the variational method, find an expression for the ground state energy of the particle. Compare the ground state energy with U_0. Is the ground state a bound one? What is the characteristic localization length of the ground state wave function? Compare it is with a.

(b) [**5 points**] Consider the same problem in two-dimensional and three-dimensional cases. Applying the variational method, draw a conclusion whether a shallow well has a bound state in these cases. **(see Hints)**

(c) [**3 points**] Consider now a *deep* potential well for which condition (5) is reversed. Does it have a bound state in one, two, and three dimensions? What is the characteristic energy of the ground state (in terms of U_0)?

3. [**5 points**] Let us consider the energy functional of a quantum particle:

$$H\{\psi(x)\} = \int dx \, [\frac{\hbar^2}{2m}|\psi'(x)|^2 + V(x)|\psi(x)|^2], \tag{6}$$

where the first term represents the kinetic energy and the second term the potential energy.

By applying the calculus of variations, show that the wave function $\psi_0(x)$ that minimizes functional (6) satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi_0''(x) + V(x)\psi_0(x) = E_0\psi_0(x) \tag{7}$$

where E_0 is the ground state energy. When minimizing functional (6), bear in mind that there is only one particle in a state $\psi(x)$, thus the wave function $\psi(x)$ must be normalized to one:

$$\int dx \, |\psi(x)|^2 = 1. \tag{8}$$

For this reason, you need to minimize $H\{\psi(x)\}$ under constraint (8), which requires to use the Lagrange multipliers. Alternatively, you may avoid using the Lagrange multipliers by minimizing

$$H\left\{\frac{\psi(x)}{\sqrt{\int d\tilde{x}\,|\psi(\tilde{x})|^2}}\right\} \tag{9}$$

without restriction (8).

4. Consider a quantum particle of mass m moving in one dimension and interacting with a real (not complex) field $\phi(x)$, so that the total energy functional of the system is

$$H_1\{\psi(x),\phi(x)\} = \int dx \, \left\{\psi^*(x)\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \phi(x)\right]\psi(x) + \alpha\phi^2(x)\right\}, \tag{10}$$

where $\psi(x)$ is a normalized wavefunction of the particle and $\alpha \geq 0$ is a constant. The ground state of the system is determined by minimizing functional (10) with respect to both $\phi(x)$ and $\psi(x)$.

(a) [**3 points**] By applying the calculus of variations, minimize functional (10) exactly with respect to $\phi(x)$ and find the energy functional in terms of $\psi(x)$ only: $H_2\{\psi(x)\}$.

(b) [**5 points**] Use some trial function $\psi(x)$ to minimize $H_2\{\psi(x)\}$. What are the energy of the ground state, the width of the wave function $\psi(x)$, the width and the depth of the corresponding potential $\phi(x)$?

(c) [**5 points**] Apply variational approach to the same problem in two and three dimensions. Is there a bound state in these cases? If so, what are its characteristics?

(d) [**5 points**] Using the calculus of variations, find an exact equation for the function $\psi_0(x)$ that minimizes $H_2\{\psi(x)\}$.

(e) [**7 points**] Solve this equation exactly in one-dimensional case and find $\psi_0(x)$. The integrals that appear in the solution can be taken exactly. If you don't know how to calculate them, consult tables of indefinite integrals. Compare your results with the solution of Problem 4b.

In solid state physics, the field $\phi(x)$ may represent phonons, $\psi(x)$ electrons, and functional (10) the electron-phonon interaction. A bound state of the electron and the phonon field is called a polaron*. From mathematical point of view, it is a* soliton*, a localized solution of non-linear differential equations.*

Hints and Comments

2b In this problem, you are required to present only naive variational conclusions. Technically, the variational method *can* prove the *existence* of a bound state, but *cannot* prove the *absence* of a bound state. The variational conclusion about existence of a bound state in a shallow well is correct in three-dimensional case, but is wrong in two dimensions. This can be shown using different methods.

4e

$$\int \frac{dx}{\sqrt{x^2 - a^2}} = \operatorname{arccosh}\left|\frac{x}{a}\right| \tag{11}$$