

PHY662, Spring 2004, Feb. 10, 2004

17th February 2004

1 Miscellaneous

1. HWK #6 will be handed out by Thursday.
2. Read Ch. 16, but skip the path integral section.
3. Review exam.
4. Review HWK #5.
5. Variational method - another example.

2 Variational method

For an arbitrary time-independent spin-1/2 Hamiltonian, diagonalization gives the two energy eigenvalues and we are done. The vector space of interest is finite-dimensional. Once we go back to indices that are continuous, like x , or have *many* possibilities, solving problems exactly is not always possible.

One of the approximations one can make is to choose a plausible family of wavefunctions $\psi(x, \alpha, \beta, \dots)$ and optimize over the parameters α, β, \dots to estimate the ground state wave function and energy.

The principle is simple, as explained in Shankar:

- Any wavefunction provides an upper bound on the ground state energy E_0 . So varying over possibilities provides an upper bound to the ground state energy.
- All energy eigenvectors, ψ_0, ψ_1, \dots are stationary points for $\langle \mathcal{H} \rangle$.

Note that getting the wavefunction correct to order δ gives the ground state energy to accuracy δ^2 .

Also note that the variational method is generally uncontrolled: we can not always bound the errors. *Lower bounds* for the ground state energy are not always available, either.

The variational method has the advantage that it is always available for use, unlike perturbation theory.