B7.3 Further Quantum Theory Sheet 3 — HT21

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3.1 Anharmonic oscillator

The one-dimensional anharmonic oscillator has Hamiltonian

$$H_{\rm AHO} = \frac{P^2}{2m} + \frac{m\omega^2}{2}X^2 + \lambda \frac{m^2\omega^3}{\hbar}X^4 , \qquad \lambda \ll 1 .$$

1. (a) Derive the leading perturbative correction in λ to the ground state energy and the ground state itself. You should find

$$E_0^{(1)} = \frac{3}{4}\hbar\omega$$
, $|\psi_0^{(1)}\rangle = -\frac{3}{2^{3/2}}|\psi_2\rangle - \frac{3^{1/2}}{2^{5/2}}|\psi_4\rangle$.

You should, of course, use the formalism of ladder operators α_{\pm} as on problem sheet 1. Don't do any integrals!

- (b) Now find the general result for the first-order corrections $E_n^{(1)}$ and $\psi_n^{(1)}$ for general n > 0. This could get messy fast, so you should think in advance about a good way to organize your calculations. It will help to remember that $\alpha_+\alpha_- = N$ acts according to $N|\psi_n\rangle = n|\psi_n\rangle$.
- 2. Now consider the *two-dimensional* harmonic oscillator perturbed by an anharmonic coupling,

$$H_{\rm AHO_{2d}} = \frac{P_1^2 + P_2^2}{2m} + \frac{1}{2}m\omega^2(X_1^2 + X_2^2) + \lambda \frac{m^2\omega^3}{\hbar}X_1^2X_2^2 , \qquad \lambda \ll 1 .$$

In this case you may recall that the unperturbed system has non-trivial degeneracy for each energy level other than the ground state.

- (a) Compute the corrections to the ground state energy and wavefunction to first order in λ using non-degenerate perturbation theory.
- (b) Now find the first-order corrections to the second, third, and fourth energy levels. (These are degenerate levels, so you need to implement first-order degenerate perturbation theory and find how the previously degenerate states are split).

Observe how much degeneracy persists at these levels to this order. Explain as much of the remaining degeneracy as you can using discrete symmetries of the Hamiltonian.

3.2 Degenerate perturbation theory at second order

In the case of a degenerate energy level, the first-order corrections to the corresponding eigenstates are given by

$$|\psi_k^{(1)}\rangle = \sum_{m:E_m^{(0)} \neq E_k^{(0)}} \frac{\langle \psi_m^{(0)} | H^{(1)} | \psi_k^{(0)} \rangle}{E_k^{(0)} - E_m^{(0)}} \psi_m^{(0)} + \sum_{\substack{r:E_r^{(0)} = E_k^{(0)} \\ \psi_r^{(0)} \perp \psi_k^{(0)}}} \lambda_r \psi_r^{(0)} ,$$

where $\psi_k^{(0)}$ is chosen to diagonalize the restriction of $H^{(1)}$ to the degenerate eigenspace.

1. By formulating an appropriate solvability criterion for the *second-order* correction to the eigenstate, $\psi_k^{(2)}$, find an expression for the coefficients λ_r .

Under what conditions does your answer determine the coefficients?

2. Apply your result to the analysis of the *third energy level* (unperturbed energy $E = 3\hbar\omega$) of the anharmonically coupled oscillators from problem **3.1**.

Which perturbed states can you now determine unambiguously at first order? (You don't need to actually determine their form, though if interested you may want to do so.)

3.3 Variational Method

We want to explore the application of the variational method in a few examples. In each case below, use the variational Ansatz given to bound/estimate the ground state energy of the stated system.

- 1. Harmonic oscillator (with potential $V(x) = \frac{1}{2}m\omega^2 X^2$) with variational Ansatz $\psi_{\alpha}(x) \sim \exp(-\alpha x^2), \ \alpha \in \mathbb{R}.$
- 2. Harmonic oscillator with variational Ansatz $\psi_a(x) \sim \frac{1}{x^2+a^2}, a \in \mathbb{R}$. Not every Ansatz is a good one!
- 3. Particle in a box (the interval $-a \leq x \leq a$) with trial functions $\psi_n(x) \sim (a^2 x^2)^n$ for n = 1, 2, 3. These will give you a few upper bounds on the ground state energy.

Compare to the exact answer.

If you are interested and adventurous, try to consider the case $\psi_{\lambda}(x) \sim (a^2 - x^2)^{\lambda}$ for continuous λ and optimize. You can get to within .3% of the exact answer this way!