Loengud 14-16

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Question 4

Derive the system of linear equations for first-order corrections to energy and zero-order corrections to wave function. Secular equation.

Answer

We consider the perturbation theory for a system with degenerate unperturbed states $\{\psi_k^{(0)}\}$, with unperturbed energy $E^{(0)}$.

Perturbed Hamiltonian:

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}'$$

Expansion:

$$\psi = \psi^{(0)} + \lambda\psi^{(1)} + \dots, \quad E = E^{(0)} + \lambda E^{(1)} + \dots$$

Substitute into Schrödinger equation and collect first-order terms:

$$\left(\hat{H}_0 - E^{(0)}\right)\psi^{(1)} + \left(\hat{H}' - E^{(1)}\right)\psi^{(0)} = 0$$

Projecting onto the unperturbed degenerate basis $\psi_n^{(0)}$, we get:

$$\sum_k \left(H'_{nk} - E^{(1)}\delta_{nk}\right)c_k = 0$$

This leads to a homogeneous system of linear equations:

$$\sum_k \left(H'_{nk} - E^{(1)}\delta_{nk}\right)c_k = 0$$

Secular Equation:

$$\det\left|H'_{nk} - E^{(1)}\delta_{nk}\right| = 0$$

Solving this determinant equation yields the allowed first-order energy corrections $E^{(1)}$. The corresponding eigenvectors give the linear combination coefficients for the corrected wave functions.

Question 7

33

For equations:

$$\text{a) } \hat{H}_0 \varphi_n^0 = E_n^0 \varphi_n^0 \qquad \text{b) } i\hbar \frac{d}{dt} \psi_n^0 = \hat{H}_0 \psi_n^0$$

How does the solution for (b) look in the stationary case? What is the relation between wavefunctions φ_n^0 and ψ_n^0? What is the representation of the wavefunction in the case of a time-dependent perturbation:

$$i\hbar \frac{d}{dt} \psi_n(t) = \left(\hat{H}_0 + \hat{H}'(t) \right) \psi_n(t)$$

Answer

The solution to (b) in the stationary case is:

$$\psi_n^0(t) = \varphi_n^0 \cdot e^{-iE_n^0 t/\hbar}$$

This shows that the time-dependent wave function is the stationary wave function multiplied by a phase factor. Therefore,

$$\boxed{\psi_n^0(t) = \varphi_n^0 e^{-iE_n^0 t/\hbar}}$$

In the case of a time-dependent perturbation:

$$i\hbar \frac{d}{dt} \psi_n(t) = \left(\hat{H}_0 + \hat{H}'(t) \right) \psi_n(t)$$

We expand $\psi_n(t)$ in the unperturbed eigenbasis:

$$\psi_n(t) = \sum_k c_k(t) \varphi_k^0 e^{-iE_k^0 t/\hbar}$$

This converts the time-dependent Schrödinger equation into a system of differential equations for the time-dependent coefficients $c_k(t)$, which can be solved using perturbation theory.

Question 15

What is the difference between the classical Schrödinger and Dirac equations?

Answer

The main differences between the Schrödinger and Dirac equations arise from the fact that one is non-relativistic and the other is relativistic.

20

1. Schrödinger Equation (Non-Relativistic)

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi(\mathbf{r}, t)$$

Key features:

- Describes particles moving at speeds much less than the speed of light.
- Scalar equation — wavefunction ψ is a single complex-valued function.
- Does not account for spin or relativistic effects.
- Predicts negative kinetic energies for large momenta (nonphysical in high-energy regime).

2. Dirac Equation (Relativistic)

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = \left[-i\hbar c\, \boldsymbol{\alpha} \cdot \nabla + \beta m c^2 \right] \Psi(\mathbf{r}, t)$$

Description for parameters?

Key features:

- Fully relativistic — consistent with special relativity.
- Wavefunction Ψ is a four-component spinor (describes spin-$\frac{1}{2}$ particles like electrons).
- Naturally includes spin and predicts electron magnetic moment.
- Predicts existence of antimatter (e.g., positron).

Conclusion

Schrödinger: valid for low-speed particles, no spin.Dirac: valid for high-speed particles, includes spin and rela