UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

24 April 2019, 10.30 to 12.30

THEORETICAL PHYSICS 2

Answer ***all four*** *questions.*

The approximate number of marks allotted to each part of a question is indicated in the right margin where appropriate.

The paper contains five sides and is accompanied by a booklet giving values of constants and containing mathematical formulae which you may quote without proof.

You may not start to read the questions printed on the subsequent pages of this question paper until instructed that you may do so by the Invigilator.

V7.1

A

1 (a) For a spin in a magnetic field that is described by the Hamiltonian $H = -\gamma \mathbf{B} \cdot \mathbf{S}$, find the Heisenberg equations of motion $\frac{d\mathbf{S}}{dt} = \frac{i}{\hbar}[H, \mathbf{S}]$ that $\mathbf{S}(t) = e^{iHt/\hbar}\mathbf{S}e^{-iHt/\hbar}$ obeys.

[*You may find useful the commutation relations* $[S_j, S_k] = i\hbar\varepsilon_{jkl}S_l$.] [6]

(b) For a spin-1/2 the following expression holds

$$\exp(-i\boldsymbol{\theta} \cdot \mathbf{S}/\hbar) = \mathbb{1}\cos(\theta/2) - i\,\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}\sin(\theta/2) \ ,$$

where $\hat{\mathbf{n}}$ is a unit vector, $\boldsymbol{\theta} = \theta\hat{\mathbf{n}}$, and $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$, the latter being the Pauli matrices. Demonstrate its validity for $\hat{\mathbf{n}} = (1, 0, 0)$. [4]

(c) Consider an electron in a hydrogen atom under the influence of an homogeneous, pulsed electric field along the x-direction. The system is described by the Hamiltonian,

$$H(t) = H_0 + \mathcal{E}\hat{x}\,\tau\sum_{n=0}^{\infty}\delta(t - n\tau) \ ,$$

where H_0 is the Hamiltonian for the electron in the unperturbed hydrogen atom, $\mathcal{E}$ is the electric field magnitude, and τ is the time between pulses.

Limiting the Hilbert space to the one spanned by just two hydrogenic orbitals, $|1s\rangle = c_s^\dagger|0\rangle$ and $|2p_x\rangle = c_x^\dagger|0\rangle$ (where $|0\rangle$ is the vacuum state), the Hamiltonian can be written as

$$H(t) = \Delta(c_x^\dagger c_x - c_s^\dagger c_s) + \mathcal{E}x_0(c_x^\dagger c_s + c_s^\dagger c_x)\,\tau\sum_{n=0}^{\infty}\delta(t - n\tau) \ ,$$

where $\Delta = \langle 2p_x|H_0|2p_x\rangle = -\langle 1s|H_0|1s\rangle$ and $x_0 = \langle 2p_x|\hat{x}|1s\rangle = \langle 1s|\hat{x}|2p_x\rangle$.

Show that the evolution operator from just before the first pulse to just before the $(N+1)^{\text{th}}$, is given by

$$U(N\tau - \epsilon, -\epsilon) = (U_\Delta U_\mathcal{E})^N \ ,$$

where

$$U_\Delta = \begin{pmatrix} e^{i\tau\Delta/\hbar} & 0 \\ 0 & e^{-i\tau\Delta/\hbar} \end{pmatrix}, \qquad U_\mathcal{E} = \begin{pmatrix} \cos\Phi_\mathcal{E} & -i\sin\Phi_\mathcal{E} \\ -i\sin\Phi_\mathcal{E} & \cos\Phi_\mathcal{E} \end{pmatrix}$$

and $\Phi_\mathcal{E} = \mathcal{E}x_0\tau/\hbar$. [7]

(d) Apply the expression in (b) to the evolution operator in (c) for $N = 1$ to find θ and $\mathbf{n}$. Interpret this result in terms of position and momentum of the electron before the second pulse.

[*The matrix of the momentum operator in this basis is proportional to* σ_y.]

[8]

Solution 1. (a) Bookwork (A.6 in Appendix). For $H = -\gamma \mathbf{B} \cdot \mathbf{S}$. [6]

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{S} \quad = \quad \frac{i}{\hbar}[H, \mathbf{S}] = -\frac{i\gamma}{\hbar} B_j [S_j, S_k] \hat{\mathbf{e}}_k = -\frac{i\gamma}{\hbar} B_j i\hbar \varepsilon_{jkl} S_l \hat{\mathbf{e}}_k = -\gamma \mathbf{B} \wedge \mathbf{S}.$$

(b) We need to demonstrate that

$$e^{-i\theta S_x} = \mathbb{1} \cos(\theta/2) - i\sigma_x \sin(\theta/2) \ ,$$

where $S_x = \frac{1}{2}\sigma_x$. For that

$$e^{-i\theta S_x} = e^{-i\sigma_x \theta/2} = \mathbb{1} - i(\theta/2)\sigma_x - \frac{(\theta/2)^2}{2!}\sigma_x^2 + i\frac{(\theta/2)^3}{3!}\sigma_x^3 + \cdots \ ,$$

and using $\sigma_x^2 = \mathbb{1}$,

$$e^{-i\theta S_x} = \left(\mathbb{1} - \frac{(\theta/2)^2}{2!} + \frac{(\theta/2)^4}{4!} + \cdots\right) - i\left(\theta/2 - \frac{(\theta/2)^3}{3!} + \frac{(\theta/2)^5}{5!} \cdots\right)\sigma_x \ ,$$

which gives the sought expression. [4]

(c) The overall evolution is obtained by compounding a cycle consisting of a pulse with evolution $U_{\mathcal{E}}$ followed by an evolution with the operator U_Δ.

$U_\Delta = e^{-iH_0\tau/\hbar} = e^{i\tau\Delta\sigma_z/\hbar}$, and $U_{\mathcal{E}} = e^{-i\Phi_{\mathcal{E}}\sigma_x}$, followed by computation of the matrix exponentials, for the latter using the result of (b). [7]

(d)

$$U_\Delta U_{\mathcal{E}} = \begin{pmatrix} e^{-i\tau\Delta/\hbar}\cos\Phi_{\mathcal{E}} & -ie^{-i\tau\Delta/\hbar}\sin\Phi_{\mathcal{E}} \\ -ie^{i\tau\Delta/\hbar}\sin\Phi_{\mathcal{E}} & e^{i\tau\Delta/\hbar}\cos\Phi_{\mathcal{E}} \end{pmatrix}$$

from which we can read off $\cos\theta/2 = \cos(\tau\Delta/\hbar)\cos\Phi_{\mathcal{E}}$ and the direction vector

$$\hat{\mathbf{n}} = \frac{1}{\sqrt{1 - \cos^2(\tau\Delta/\hbar)\cos^2\Phi_{\mathcal{E}}}} \begin{pmatrix} -\cos(\tau\Delta/\hbar)\sin\Phi_{\mathcal{E}} \\ \sin(\tau\Delta/\hbar)\sin\Phi_{\mathcal{E}} \\ -\sin(\tau\Delta/\hbar)\cos\Phi_{\mathcal{E}} \end{pmatrix}.$$

Interpretation: The problem in (c) maps to a problem of a precessing spin-1/2, in which θ would be the angle of precession, and $\hat{\mathbf{n}}$ the axis around which it precesses. The $+S_z$ component accounts for the degree of excitation onto the $2p_x$ orbital, while the S_x and S_y components account for the hybridisation between the $1s$ and the $2p_x$ states, with σ_x describing the displacement of the average position of the electron w.r.t. the nucleus, while σ_y describes its momentum (the momentum operator in this basis $p_x = \frac{\hbar}{i}\partial_x \propto \sigma_y$). [8]

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2 A particle of energy $E = \frac{\hbar^2 k^2}{2m}$ is scattered from a localised potential $V(\mathbf{r})$.

(a) Outline the essential elements of partial-wave analysis, leading to

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin\delta_l e^{i\delta_l}P_l(\cos\theta) \qquad (\dagger)$$

defining all quantities that appear in this expression. [7]

(b) Use (†) to derive the optical theorem for the total scattering cross-section

$$\sigma_{\text{tot}} = \frac{4\pi}{k}\text{Im}f(\theta = 0).$$

You may find it useful to know that $\int_{-1}^{1} P_l(x)P_{l'}(x)dx = \frac{2\delta_{ll'}}{2l+1}$ and $P_l(1) = 1$. [6]

(c) Find the phase shift $\delta_0(k)$ for the s-wave scattering as a function of the wave vector k for a hard-sphere potential $V(r) = \infty$ for $r < R$, $V(r) = 0$ for $r > R$. Determine the s-wave scattering length a_0 and the s-wave scattering amplitude f_0. Sketch the s-wave scattering cross-section $\sigma_0(k)$, choosing the appropriate dimensionless units, and discuss its (three) prominent features. [6]

(d) Find the scattering amplitude for delta-shell potential $V(\mathbf{r}) = V_0\delta(r - R)$ in the first Born approximation f_{Born}. Discuss the dependence of the scattering cross-section on the angle θ for small and large wave vector k. Does the first Born approximation you obtained in this part satisfy the optical theorem? [6]

Solution 2. (a) Bookwork. Should mention: need spherically symmetric potential $V(\mathbf{r}) = V(r)$, the conservation of angular momentum defining scattering channels for the different $l = 0, 1, \ldots$. Phase shifts $\delta_l(k)$ contain all information needed for the scattering amplitude in asymptotic solution $\psi_k(\text{r}) \to e^{ikz} + f(\theta)\frac{e^{ikr}}{r}$ for $r \to \infty$. (b) $\text{Im}f(\theta = 0) = \frac{1}{k}\sum_l(2l+1)\sin\delta_l\sin\delta_l P_l(1) = \frac{1}{k}\sum_l(2l+1)\sin^2\delta_l$. On the other hand $\sigma_{\text{tot}} = \int |f(\theta)|^2 d\Omega = \frac{2\pi}{k^2}\int_{-1}^{+1} dx \sum_{l,l'}(2l+1)(2l'+1)\sin\delta_l\sin\delta_{l'}P_l(x)P_l'(x) = \frac{4\pi}{k^2}\sum_l(2l+1)\sin^2\delta_l$. (c) Matching at $r = R$ for $u_0(R) = A\sin(kR + \delta_0) = 0$ gives $\delta_0 = -kR$ which implies $a_0 = -\delta_0/k = R$ and $\sigma_0 = \frac{4\pi R^2}{(kR)^2}\sin^2 kR$. Mention features: maximum $\sigma_0 = 4\pi R^2$ for $kR = 0$, unitarity for $kR = \pi/2$, transparency for $kR = \pi$. (d) $f(\theta) = -\frac{m}{2\pi\hbar^2}\int d\mathbf{r}e^{i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r}) = -\frac{2m}{\hbar^2 q}\int_0^\infty drV(r)\sin qr = -\frac{2mV_0 R\sin qR}{\hbar^2 q}$. Say $f(\theta)$ is a function of $q^2 = 2k^2(1-\cos\theta)$ only, small q is $f(\theta) = -\frac{2mV_0R^2}{\hbar^2}$ independent of θ (s-wave scattering), large q is $f(\theta) \to 0$, $f(\theta)$ is real, optical theorem does not hold.

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3 (a) State the algebraic relations that creation and annihilation operators satisfy for bosons (fermions). Write down the number operators for bosons (fermions) and their possible eigenvalues for bosons (fermions). [5]

Consider the following Hamiltonian describing two interacting spins 1/2

$$H = -J\left(\hat\sigma_1^x\hat\sigma_2^x + \hat\sigma_1^y\hat\sigma_2^y\right) - h\left(\hat\sigma_1^z + \hat\sigma_2^z\right) \qquad (\star)$$

where $\hat\sigma_j^\alpha$ with $\alpha = x, y, z$ and $j = 1, 2$ are the standard Pauli matrices.

(b) Given the raising ($\hat\sigma_j^+$) and lowering ($\hat\sigma_j^-$) operators, $\hat\sigma_j^\pm = \hat\sigma_j^x \pm i\hat\sigma_j^y$, find the eigenvalues and eigenvectors of the Hamiltonian ($\star$). [4]

In one dimension one can rewrite spins in terms of fermionic operators

$$\hat\sigma_1^- = \hat f_1, \quad \hat\sigma_2^- = e^{i\pi \hat f_1^\dagger \hat f_1}\hat f_2, \quad \hat\sigma_j^z = 2\hat f_j^\dagger \hat f_j - 1$$

where $\hat f_j$ with $j = 1, 2$ are the standard fermionic annihilation operators.

(c) Use algebraic relations for fermionic operators to obtain the commutators

$$\left[\hat\sigma_1^-, \hat\sigma_1^+\right], \quad \left[\hat\sigma_1^z, \hat\sigma_2^z\right], \quad \left[\hat\sigma_1^-, \hat\sigma_2^-\right], \quad \left[\hat\sigma_2^-, \hat\sigma_2^+\right],$$

and show that they are consistent with the spin angular momentum algebra. [8]

(d) Now rewrite the Hamiltonian ($\star$) in terms of fermionic operators and find the eigenvalues and eigenstates by diagonalising this bilinear Hamiltonian. [8]

Solution 3. (b) With $\hat\sigma_j^\pm = \hat\sigma_j^x \pm i\hat\sigma_j^y$ get $H = -\frac{J}{2}\left(\hat\sigma_1^-\hat\sigma_2^+ + \hat\sigma_1^+\hat\sigma_2^-\right) - h\left(\hat\sigma_1^z + \hat\sigma_2^z\right)$. Total magnetisation is conserved $[\hat\sigma_1^z + \hat\sigma_2^z, H] = 0$. Eigenvalues $-2h$ for $|\downarrow\downarrow\rangle$, $\mp\frac{J}{2}$ for $\frac{|\downarrow\uparrow\rangle \pm |\downarrow\uparrow\rangle}{\sqrt{2}}$, $+2h$ for $|\uparrow\uparrow\rangle$. (a) Bookwork. $[\hat a_i, \hat a_j]_\mp = 0 = [\hat a_i^\dagger, \hat a_j^\dagger]_\mp$ and $[\hat a_i, \hat a_j^\dagger]_\mp = \delta_{ij}$ $\hat n_j = \hat a_j^\dagger \hat a_j$ with $n_j = 0, 1$ fermions and $n_j = 0, 1, 2, \dots$ bosons. (d) As $\hat f_1^\dagger e^{i\pi \hat f_1^\dagger \hat f_1} = \hat f_1^\dagger$ we get $H = -\frac{J}{2}\left(\hat f_1^\dagger \hat f_2 + \hat f_2^\dagger \hat f_1\right) - 2h\left(\hat f_1^\dagger \hat f_1 + \hat f_2^\dagger \hat f_2\right) + 2h$. Using $\hat c_\pm = \frac{\hat f_1 \pm \hat f_2}{2}$ we get $H = \left(-2h - \frac{J}{2}\right)\hat c_1^\dagger \hat c_1 + \left(-2h + \frac{J}{2}\right)\hat c_2^\dagger \hat c_2 + 2h$. Eigenvalues $+2h$ for $|0,0\rangle$, $\frac{J}{2}$ for $|1,0\rangle$, $-\frac{J}{2}$ for $|0,1\rangle$, $-2h$ for $|0,0\rangle$. As expected, we get the same spectrum as in part (a). (c) Use fermionic anti-commutation relations, $\hat f_1 e^{i\pi \hat f_1^\dagger \hat f_1} = -\hat f_1$, and $e^{i\pi \hat f_1^\dagger \hat f_1}\hat f_1 = +\hat f_1$.

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4 (a) Define the density operator $\hat{\rho}$ of a quantum system that has probability p_i to be in each of the normalised states $|\psi_i\rangle$. Explain the distinction between mixed and pure states of a quantum system, and how this distinction is reflected in the density matrix. [4]

(b) Experimentalist A prepares a stream of atoms such that each atom is in state $|\psi_A\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Experimentalist B prepares a stream of atoms which is a mixture: half the atoms are in state $|\uparrow\rangle$ and half are in state $|\downarrow\rangle$. In the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ determine the density matrices ρ_A and ρ_B. [6]

(c) Show that streams A and B cannot be distinguished by making a measurement of σ_z, but that they can be told apart by measuring σ_x. [3]

(d) Experimentalist C prepares a stream which is an equal mixture of atoms in the two states $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$. Can this be distinguished from streams A and B, and, if so, how? [3]

(e) Experimentalist D produces two streams of atoms flying in opposite directions, in such away that each atom flying to the left is entangled with another flying to the right, both forming a singlet of wavefunction

$$|\psi_D\rangle = \frac{1}{\sqrt{2}}(|\uparrow_L\downarrow_R\rangle - |\downarrow_L\uparrow_R\rangle) ,$$

in an experiment analogous to the one proposed by Einstein, Podolsky and Rosen in 1935. In the basis $\{|\uparrow_L\uparrow_R\rangle, |\uparrow_L\downarrow_R\rangle, |\downarrow_L\uparrow_R\rangle, |\downarrow_L\downarrow_R\rangle\}$: (*i*) compute the density matrix and check it corresponds to a pure state. (*ii*) Extract from it the reduced density matrix for measurements on the right stream, and (*iii*) calculate its entanglement entropy. [6]

(f) A stream prepared by experimentalist E is thermally equilibrated in a magnetic field $\mathbf{B} = (0, 0, B_z)$ at temperature T. The atoms have magnetic moment μ. Determine the density matrix ρ_E. [3]

Solution 4. (a) The density operator is defined by $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ where p_i is the probability of the system being in state $|\psi_i\rangle$. [2]

The maximum information which can be obtained on a system consists of the eigenvalues of the complete set of commuting observables. The states of maximum knowledge are called pure states. If a quantum mechanical system is in a pure state, it can be characterised by a single state vector, i.e. $p_i = 1$ for one value of i in the above equation, and $p_i = 0$ for all other states. In a mixed state, the system cannot be characterised by a single state vector, but may be described as having certain probabilities $p_i < 1$ of being in each of the pure states $|\psi_i\rangle$. The density matrix would show $\mathrm{tr}\,\rho^2 = 1$ for pure states and $\mathrm{tr}\,\rho^2 < 1$ for mixed states. [2]

(b)

$$\rho_A = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)\frac{1}{\sqrt{2}}(\langle\uparrow + \langle\downarrow|) = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}$$

$$\rho_B = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| = \frac{1}{2}\begin{pmatrix}1\\ 0\end{pmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \frac{1}{2}\begin{pmatrix}0\\ 1\end{pmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

[6]

(c) For stream A

$$\langle\sigma_z^A\rangle = \mathrm{tr}[\rho_A\sigma_z] = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = 0\,,$$

$$\langle\sigma_x^A\rangle = \mathrm{tr}[\rho_A\sigma_x] = \frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = 1\,,$$

For stream B, $\rho_B \propto \mathbb{1}$ and the Pauli matrices have zero trace, so $\langle\sigma_z^B\rangle = \langle\sigma_x^B\rangle = 0$. Therefore, streams A and B can be distinguished by measuring $\langle\sigma_x\rangle$, but not $\langle\sigma_z\rangle$. [3]

(d) $\rho_C = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \rho_B$. Therefore, C cannot be distinguished from B by any measurement, but can be told apart from A by measuring $\langle\sigma_x\rangle$. [3]

(e)

$$\rho = \frac{1}{2}(|\uparrow_L\downarrow_R\rangle - |\downarrow_L\uparrow_R\rangle)(\langle\uparrow_L\downarrow_R| - \langle\downarrow_L\uparrow_R|) = \frac{1}{2}\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 1 & -1 & 0\\ 0 & -1 & 1 & 0\\ 0 & 0 & 0 & 0\end{pmatrix}$$

$$\rho^2 = \frac{1}{4}\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 2 & -2 & 0\\ 0 & -2 & 2 & 0\\ 0 & 0 & 0 & 0\end{pmatrix} = \rho$$

and, therefore, $\mathrm{tr}\,\rho^2 = 1$, as it should for a pure state.

The reduced density matrix is

$$\rho_R^{\mathrm{red}} = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

and the entanglement entropy $S = -k\sum_n p_n \log p_n = -2k(\frac{1}{2}\log\frac{1}{2}) = k\log 2$. [6]

(f) At thermal equilibrium with $\beta = 1/kT$ [3]

$$\rho_E = \frac{1}{2\cosh(\beta\mu B_z)}\begin{pmatrix}e^{\beta\mu B_z} & 0\\ 0 & e^{-\beta\mu B_z}\end{pmatrix}.$$

in the basis of eigenstates of S_z.

END OF PAPER