

26 April 2017, 10.30 to 12.30

THEORETICAL PHYSICS 2

*Answer **all four** questions. Each question consists of 5 parts, worth 5 marks each. 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.

1 In second quantization two-body interactions $U(x, x')$ can be described by

$$\hat{H}_{\text{int}} = \frac{1}{2} \int dx dx' \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') U(x, x') \hat{\psi}(x') \hat{\psi}(x).$$

(a) Which algebraic relations do the operators $\hat{\psi}(x)$ satisfy for bosons (fermions)? Which algebraic relations do the creation and annihilation operators, \hat{a}_α^\dagger and \hat{a}_α , in some orthonormal single-particle basis $\{\varphi_\alpha(x)\}$ satisfy for bosons (fermions)? How are the number operators defined? What are their possible eigenvalues for bosons (fermions)?

(b) Consider as the single-particle basis, two orthonormal eigenfunctions of a uniform 1D ring of length L , i.e. $\varphi_1(x) \propto e^{ik_1x}$ and $\varphi_2(x) \propto e^{ik_2x}$. Show that the bosonic Hamiltonian for the interaction potential $U(x, x') = g\delta(x - x')$ is

$$\hat{H}_{\text{int}} = \alpha \hat{n}_1(\hat{n}_1 - 1) + \beta \hat{n}_2(\hat{n}_2 - 1) + \gamma \hat{n}_1 \hat{n}_2 \quad (\star)$$

where \hat{n}_1 and \hat{n}_2 are number operators corresponding to single-particle states $|\varphi_1\rangle$ and $|\varphi_2\rangle$ with real-space wavefunctions $\varphi_1(x)$ and $\varphi_2(x)$, respectively.

(c) Find the ground state of (\star) for a fixed total number, $\hat{n}_1 + \hat{n}_2 = N$, and repulsive interactions $g > 0$. If you have not solved (b), then find the ground state of (\star) for $\alpha = \beta < 0$ and $\gamma = 0$, and a fixed total number, $\hat{n}_1 + \hat{n}_2 = N$.

(d) How would you take into account dispersion, i.e. that the energies of the two single-particle states $\varphi_1(x)$ and $\varphi_2(x)$ could be different? Write down the Hamiltonian including dispersion and its explicit matrix for $N = 2$ bosons. Find the ground state of this Hamiltonian for repulsive interactions $g > 0$.

(e) Consider as the single-particle basis, two orthonormal eigenfunctions of 1D box potential of length L , i.e. $\varphi_1(x) \propto \sin k_1x$ and $\varphi_2(x) \propto \sin k_2x$. Find the Hamiltonian for the interaction potential $U(x, x') = g\delta(x - x')$ as in (b). Which feature complicates your finding of the ground state similar to (c)?

Solution 1. (a) Bookwork. (b) Using the expansion $\hat{\psi}(x) = \varphi_1(x)\hat{a}_1 + \varphi_2(x)\hat{a}_2$ we obtain the Hamiltonian $\hat{H}_{\text{int}} = \frac{1}{2} \sum_{klmn} U_{klmn} a_k^\dagger a_l^\dagger a_m a_n$. The non-zero elements are $U_{1111} = U_{2222} = g$, $U_{1212} = U_{1221} = U_{2112} = U_{2121} = g$ for the single-particle states, so $\hat{H}_{\text{int}} = \frac{g}{2L} [\hat{n}_1(\hat{n}_1 - 1) + \hat{n}_2(\hat{n}_2 - 1) + 4\hat{n}_1\hat{n}_2]$. (c) Using $\hat{n}_2 = N - \hat{n}_1$ we get $\hat{H}_{\text{int}} = \frac{g}{2L} [N^2 - N + 2\hat{n}_1(N - \hat{n}_1)]$ so ground state twofold degenerate $|N, 0\rangle$, $|0, N\rangle$. For $\alpha = \beta < 0$ and $\gamma = 0$, $\hat{H}_{\text{int}} = \alpha [N^2 - N - 2\hat{n}_1(N - \hat{n}_1)]$ with the same ground states. (d) $\hat{H} = E_1\hat{n}_1 + E_2\hat{n}_2 + \hat{H}_{\text{int}}$ which is diagonal. For $N = 2$, this is a 3×3 matrix. For $E_2 - E_1 > 0$ it is $|N, 0\rangle$, for $E_2 - E_1 < 0$ it is $|0, N\rangle$. (e) The overlap integrals can be done using $2\sin^2 \frac{x}{2} = 1 - \cos x$ and orthogonality of $\cos mx$. The complication is that \hat{H}_{int} is not diagonal in this basis: it contains terms $\hat{a}_1^\dagger \hat{a}_1^\dagger \hat{a}_2 \hat{a}_2$ with a coefficient $\int_0^L dx \sin^2 k_n x \sin^2 k_m x = \frac{L}{4}(1 + \frac{1}{2}\delta_{mn})$.

V7.1

- 2 Consider the Hamiltonian of a harmonic oscillator with an external force F

$$H = \frac{p^2}{2M} + \frac{M\omega^2 x^2}{2} - Fx. \quad (**)$$

- (a) Give the eigenstates and the eigenenergies of the Hamiltonian (**).
- (b) What is the definition of the coherent state $|\alpha\rangle$? What is its position uncertainty? Show that $|\alpha\rangle$ is the displaced vacuum, i.e. $|\alpha\rangle = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}|0\rangle$, where $|0\rangle$ is the ground state of the oscillator.
- Hint:* For $[A, B] = \alpha$ we have $e^A e^B = e^{A+B} e^{\alpha/2} = e^B e^A e^\alpha$.
- (c) Assuming the system is in the ground state for $F = 0$ at time $t = 0$, when the force is suddenly switched on $F = F_0$, what is the state at the time $t > 0$?

A particle with spin $\frac{1}{2}$ is in thermal equilibrium with a thermal bath at absolute temperature T and under the influence of constant magnetic field \mathbf{B} .

- (d) Write down the density operator ρ describing the spin $\frac{1}{2}$ in this situation. In which limit is the state of the system pure? When is it maximally mixed? In which situation would the notion of negative temperatures make sense?
- (e) Calculate the expectation value of the spin component \hat{S}_z for $\mathbf{B} = B\mathbf{e}_z$. Sketch the dependence of your result as a function of (inverse) temperature.

Solution 2. (a) Completing the square $H = \frac{p^2}{2M} + \frac{M\omega^2}{2}(x - x_0)^2 - \frac{F_0^2}{2M\omega^2}$, we find the eigenstates are displaced oscillator states with $E_n = \hbar\omega n - \frac{F_0^2}{2M\omega^2}$ and $x_0 = \frac{F_0}{m\omega^2}$. (b) Bookwork. $\hat{a}|\alpha\rangle = \alpha|\alpha\rangle$. $\langle\alpha|\hat{x}^2|\alpha\rangle - \langle\alpha|\hat{x}|\alpha\rangle^2 = x_{\text{ZPF}}^2$. (c) From part (a), we know that the initial state is a coherent state $|\psi(t=0)\rangle = |\alpha_0\rangle$ with $\alpha_0 = \frac{F_0 x_{\text{ZPF}}}{\hbar\omega}$ so the dynamics is $|\psi(t)\rangle = |e^{-i\omega t}\alpha_0\rangle$. (d) $\rho = \frac{1}{Z}e^{-\beta H}$ and $Z = \text{tr } \rho$ and $H = -\gamma\mathbf{B} \cdot \mathbf{S}$. Negative temperatures correspond the spin pointing in the opposite direction. (e) $\langle\hat{S}_z\rangle = \text{tr } \hat{S}_z \rho = \frac{\hbar}{2} \frac{e^{-\gamma\beta B} - e^{+\gamma\beta B}}{e^{-\gamma\beta B} + e^{+\gamma\beta B}}$, i.e. pure state $T \rightarrow 0$ and totally mixed $T \rightarrow \infty$.

(a) Show that the propagator of a one-dimensional time-independent Hamiltonian with a complete set of energy eigenfunctions $\{\varphi_\alpha(x)\}$ and eigenvalues $\{E_\alpha\}$ is

$$K(x, t|x', t') = \theta(t - t') \sum_{\alpha} \varphi_{\alpha}(x) \varphi_{\alpha}^{*}(x') e^{-iE_{\alpha}(t-t')/\hbar}.$$

(b) The Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - g\delta(x)$$

describes an attractive δ -function potential ($g > 0$). There is a single bound state of the form

$$\varphi_0(x) = \sqrt{\kappa} e^{-\kappa|x|}.$$

Find κ and the energy E_0 of the bound state.

(c) Find the phase shifts $\delta_{\text{even}}(k)$ and $\delta_{\text{odd}}(k)$ for scattering in the even and odd channels at wavevector k .

(d) Show that the propagator $K(0, T|0, 0)$ can be written

$$K(0, T|0, 0) = \kappa e^{-iE_0 T/\hbar} + \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{k^2}{\kappa^2 + k^2} \exp\left(-\frac{i\hbar k^2 T}{2m}\right). \quad (\star \star \star)$$

(e) How does the expression $(\star \star \star)$ behave as $T \rightarrow \infty$?

Solution 3.

(a) The propagator is

$$K(x, t|x', t') = \theta(t - t') \langle x|U(t, t')|x'\rangle.$$

Writing

$$U(t, t') = e^{-iH(t-t')/\hbar} = \sum_{\alpha} |\varphi_{\alpha}\rangle \langle \varphi_{\alpha}| e^{-iE_{\alpha}(t-t')/\hbar}$$

and taking matrix elements gives the answer.

(b) This is a question of substituting in

$$\partial_x^2 \varphi_0(x) = \kappa^2 \varphi_0(x) + 2\kappa \delta(x),$$

from which we get $\kappa = gm/\hbar^2$ and $E_0 = \hbar^2 \kappa^2 / 2m$.

(c) $\delta_{\text{odd}}(k) = 0$ as the odd wavefunctions vanish at the origin.

Write the even wavefunctions as

$$\psi_{k,\text{even}}(x) = \cos(k|x| - \delta_{\text{even}}(k)).$$

Apply the boundary condition

$$\frac{\hbar^2}{2m} \psi'(x)|_{-}^{+} = -g\psi(0)$$

gives

$$\frac{\hbar^2 k}{m} \sin \delta_{\text{even}} = g \cos \delta_{\text{even}}$$

or

$$\tan \delta_{\text{even}} = \kappa/k.$$

(d) This is a matter of substituting the results of (b) and (c) into the formula from part (a). The odd channel doesn't contribute. Each state in the even channel contributes

$$\cos^2 \delta_{\text{even}} = \frac{k^2}{k^2 + \kappa^2}.$$

The correct numerical factor requires a density of states calculation.

Alternatively, the shortcut is to note that $\kappa \rightarrow 0$ should recover the free particle propagator, which fixes the factor.

(e) The best way to get at this is write the second term as

$$\left(\frac{m}{\hbar^2 T}\right)^{3/2} \int_{-\infty}^{\infty} \frac{du}{2\pi} \frac{u^2}{\kappa^2 + mu^2/(\hbar^2 T)} \exp\left(-\frac{iu^2}{2}\right).$$

Expanding the denominator and doing the integrals yields a series (actually an asymptotic series) in $T^{-m-1/2}$ for $m = 1, 2, \dots$. The behaviour at long times is thus dominated by the term $\kappa e^{-iE_0 T/\hbar}$ arising from the bound state.

4 Consider the scattering problem in two dimensions.

(a) Show that the asymptotic form of the scattered wave in this case is

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} e^{ikr \cos \theta} + \sqrt{\frac{i}{kr}} f(\theta) e^{ikr},$$

which defines the (dimensionless) scattering amplitude $f(\theta)$ in two dimensions.

$$\left[\begin{array}{l} \text{Hint: You may find it helpful to know that the form of the Laplacian in} \\ \text{polar coordinates } (r, \theta) \text{ is} \\ \\ \nabla^2 f = \frac{1}{r} \partial_r (r \partial_r f) + \frac{1}{r^2} \partial_\theta^2 f. \end{array} \right]$$

(b) Show that the total cross-section, which has the units of length, is

$$\lambda = \frac{1}{k} \int d\theta |f(\theta)|^2.$$

(c) Show that the 2D plane wave has the expansion

$$\exp(ikr \cos \theta) = \sum_{m=-\infty}^{\infty} a_m J_m(kr) e^{im\theta},$$

where $J_m(\rho)$ is the Bessel function satisfying

$$\rho^2 \frac{d^2}{d\rho^2} J_m + \rho \frac{d}{d\rho} J_m + (\rho^2 - m^2) J_m = 0,$$

and a_m are some coefficients to be determined below.

(d) Given the behaviour

$$J_m(\rho) \rightarrow \frac{\rho^m}{2^m m!} \text{ as } \rho \rightarrow 0,$$

find the coefficients a_m in the previous part.

(e) The asymptotic form of the scattered wave can be written

$$\psi_{\mathbf{k}}(\mathbf{r}) \xrightarrow{r \rightarrow \infty} \sum_{m=0}^{\infty} \sqrt{\frac{2}{\pi kr}} \epsilon_m i^m e^{i\delta_m} \cos(m\theta) \cos\left(kr - \frac{m\pi}{2} - \frac{\pi}{4} + \delta_m\right)$$

where $\epsilon_0 = 2$ and $\epsilon_{m \neq 0} = 1$. Find expressions for $f(\theta)$ and λ in terms of δ_m .

Solution 4.

(a) The given asymptotic form satisfies

$$(\nabla^2 + k^2) \psi_{\mathbf{k}} = \sqrt{\frac{i}{k}} \left(\frac{f(\theta)}{4} + f''(\theta) \right) \frac{e^{ikr}}{r^{5/2}}.$$

The remainder on the RHS will be cancelled by subleading terms in the asymptotic expansion.

(b) The non-oscillating terms in the flux

$$j = -\frac{i\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*)$$

are

$$\frac{\hbar k}{m} \hat{\mathbf{x}} + \frac{\hbar |f(\theta)|^2}{mr} \hat{\mathbf{r}}.$$

The probability / time into an angle $d\theta$ is $\propto (\hbar/m) |f(\theta)|^2 d\theta$ while the incident flux is $\propto \hbar k/m$. The cross section is the ratio

$$d\lambda = \frac{|f(\theta)|^2 d\theta}{k}.$$

Integrating over θ gives the total cross section.

(c) We look for separable solutions of the Helmholtz equation

$$[\nabla^2 + k^2] \Phi(r, \theta) = 0,$$

where

$$\nabla^2 = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}.$$

Separable solutions are then shown to have the form $\Phi(r, \theta) = J_m(kr) e^{im\theta}$. The expansion of the plane wave then follows.

(d) This follows closely the 3D case. The key point is that a term $(kr)^m e^{im\theta}$ arises only from the m^{th} order. Using the given asymptote and comparing coefficients then gives $a_m = i^m$.

(e) We have

$$i^m e^{i\delta_m} \cos \left(kr - \frac{m\pi}{2} - \frac{\pi}{4} + \delta_m \right) = \frac{1}{2} \left(\overbrace{\sqrt{-i} e^{ikr+2\delta_m}}^{\text{out}} + \overbrace{\sqrt{i} (-1)^m e^{-ikr}}^{\text{in}} \right). \quad (1)$$

The crucial part is to subtract the asymptotic form of the plane wave expansion, which corresponds to setting $\delta_m = 0$, to leave only the outgoing wave. The scattering amplitude $f(\theta)$ can then be read off as

$$f(\theta) = \sum_{m=0}^{\infty} \sqrt{\frac{2}{\pi}} \epsilon_m e^{i\delta_m} \sin \delta_m \cos(m\theta).$$

Evaluating λ gives

$$\lambda = \frac{4}{k} \sum_{m=0}^{\infty} \epsilon_m \sin^2 \delta_m.$$

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