UNIVERSITY OF CAMBRIDGE

NATURAL SCIENCES TRIPOS Part II

Wednesday 22 April 2020, 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 four sides and is accompanied by a booklet giving values of constants and containing mathematical formulae which you may quote without proof. (The booklet is available for separate download.)

Please write answers in a manner that will be suitable for scanning and uploading. You will have 30 minutes after the end of the examination to scan and upload the answers. (See coversheet for further details.)

V7.1

A

1 A particle of mass M and energy $E = \hbar^2 k^2/2M$ scatters elastically from a spherically symmetric potential $V(r)$ which is zero for $r > R_0$.

(a) State what is meant by partial wave analysis. Explain in general terms (without mathematical detail) why scattering can be encoded in terms of phase shifts. [6]

(b) Writing the wavefunction for a particle with angular momentum quantum numbers ℓ and m_ℓ as

$$\Psi(\boldsymbol{r}) = Y_{\ell,m_\ell}(\theta,\phi)\frac{u_\ell(r)}{r}$$

where (r,θ,ϕ) are spherical polar co-ordinates, and $Y_{\ell,m_\ell}(\theta,\phi)$ is the spherical harmonic, show that the function $u_\ell(r)$ satisfies [5]

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{\ell(\ell+1)}{r^2} + \frac{2M}{\hbar^2}V(r)\right]u_\ell(r) = k^2 u_\ell(r)\,.$$

[You may use $\nabla^2 = \frac{1}{r^2}\partial_r\left(r^2\frac{\partial}{\partial r}\right) - \frac{\boldsymbol{L}^2}{\hbar^2 r^2}$ where $\boldsymbol{L}^2$ is the squared total angular momentum operator.]

(c) Show that for $\ell = 0$ the function $u_0(r)$ at large radii, $r > R_0$, can be written as

$$u_0(r) \propto \sin(kr + \delta_0) \qquad (\star)$$

and explain the physical meaning of the phase shift δ_0. [5]

A certain potential has a bound state for $\ell = 0$ at an energy $E = -E_\mathrm{B}$ with E_B positive.

(d) Show that for $r > R_0$ the bound state wavefunction is of the form

$$u_0^\mathrm{B}(r) \propto e^{-\kappa r}$$

and determine the value of κ. Hence show that, for $E_\mathrm{B} \ll \hbar^2/MR_0^2$ the bound state wavefunction is mostly at $r > R_0$. [4]

(e) Assuming $E_\mathrm{B} \ll \hbar^2/MR_0^2$, use orthogonality of the scattering state $(\star)$ with $u_0^\mathrm{B}(r)$, or otherwise, to determine the phase shift δ_0 for low-energy scattering. [5]

[Hint: In this limit, you can compute the overlap by considering $R_0 \to 0$ and integrating the functions over $r = 0 \to \infty$.]

Solution 1. (a) – The potential must have spherical symmetry.
– Energy eigenstates can be classified in terms of angular momentum: Each angular momentum channel scatters without change of angular momentum.
– Conservation of flux means that for the outgoing wave in a given angular momentum channel can only differ from that with no scattering potential by a phase shift, conventionally denoted $e^{2i\delta_\ell}$. (Scattering is unitary.)
– There is one phase shift for each value of the total angular momentum ℓ.

(b) The TISE at energy $E = \hbar^2 k^2/2M$ is

$$\begin{aligned}
-\frac{\hbar^2}{2M}\nabla^2\psi + V\psi &= \frac{\hbar^2 k^2}{2M}\psi \\
\left[-\frac{1}{r^2}\partial_r\left(r^2\partial_r\right) + \frac{\boldsymbol{L}^2}{\hbar^2 r^2} + V\right]\psi &= k^2\psi \\
\boldsymbol{L}^2 Y_{\ell,m} &= \hbar^2\ell(\ell+1)Y_{\ell,m} \\
-\frac{1}{r^2}\partial_r\left(r^2\partial_r\right)\frac{u_\ell(r)}{r} + \frac{\ell(\ell+1)}{r^2}\frac{u_\ell(r)}{r} + V(r)\frac{u_\ell(r)}{r} &= k^2\frac{u_\ell(r)}{r}
\end{aligned}$$

Simple manipulations of the derivatives lead to requested result:

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \frac{2M}{\hbar^2}V(r)\right]u_\ell(r) = k^2 u_\ell(r)\,.$$

(c) For $r > R_0$

$$-\frac{d^2}{dr^2}u_0(r) = k^2 u_0(r)\,.$$

The general solution is of the form

$$u_0(r) \propto \sin(kr + \delta_0)$$

Some discussion of the interpretation of δ_0 required could include points such as:
– For no potential, $\delta_0 = 0$, required such that u_0/r is finite as $r \to 0$.
– The scattering introduces non-zero δ. Writing as:

$$u_0(r) \propto e^{-ikr} - e^{+ikr+2i\delta_0}$$

we see that the phase shift is $2i\delta_0$ on the outgoing wave.
– For low energy, $k \to 0$, the phase shift can also be interpreted as a scattering length, $\delta \to -ka$.

(d) For $r > R_0$ state of energy $E = -E_\mathrm{B}$ satisfies

$$-\frac{d^2}{dr^2}u_0 = -\kappa^2 u_0$$

with $\kappa = \sqrt{2ME_\mathrm{B}}/\hbar$.

The bound state solution must be of the form $u_0 \propto e^{-\kappa r}$, with the other wave $e^{+\kappa r}$ vanishing to allow normalization.

For $E_{\mathrm{B}} \ll \frac{\hbar^2}{MR_0^2}$ one has $1/\kappa \gg R_0$. Therefore most of the probability of the boundstate lies outside of R_0.

(e) The scattering wave must be orthogonal to this. For $E_{\mathrm{B}} \ll \hbar^2/MR_0^2$ we have $1/\kappa \gg R_0$ so most weight lies outside R_0.

Orthogonality requires

$$\int_{R_0 \simeq 0}^{\infty} \frac{\sin(kr+\delta_0)}{r} \frac{e^{-\kappa r}}{r} r^2 dr = 0$$

At low energy $\sin(kr+\delta_0) \simeq kr + \delta_0$. Hence

$$\begin{aligned} \int_0^{\infty} (kr+\delta_0) e^{-\kappa r} dr &= 0 \\ k/\kappa^2 + \delta_0/\kappa &= 0 \\ \delta_0 &= -\frac{k}{\kappa} \end{aligned}$$

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2 (a) Write the density matrix in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis for an ensemble of spin-1/2 particles in each of the following situations:

(i) each particle is in the state $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i|\downarrow\rangle)$;

(ii) an equal statistical mixture of states $|\uparrow\rangle$ and $|\downarrow\rangle$;

(iii) an equal statistical mixture of states $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$.

(b) Which of the above situations are physically distinct? What observable can be measured to differentiate them? Find the expectation of this observable from the three density matrices. [5]

[*The spin operators are described by Pauli matrices in the* $\{|\uparrow\rangle, |\downarrow\rangle\}$ *basis:*

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
]

Two spin-1/2 particles interact via the Hamiltonian

$$H = -2J(\mathbf{S}_1 \cdot \mathbf{S}_2/\hbar^2 + 1/4).$$

Writing the time-evolution operator $U(t) = e^{-iHt/\hbar}$ in the basis of states $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ gives the matrix

$$U(t) = \begin{pmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta & 0 \\ 0 & i\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix},$$

where $\theta \equiv Jt/\hbar$.

(c) Suppose we prepare the system in the state $|\uparrow\downarrow\rangle$ at $t = 0$. Find the density matrix at time t using $\rho(t) = U(t)\rho(0)U^\dagger(t)$. What pure state does it describe? [5]

(d) Find the reduced density matrix $\rho_{\text{red}}(t)$ describing the first spin by tracing over the latter. [4]

(e) Find the entanglement entropy $S_{\text{ent}}(t)$ from the eigenvalues of ρ_{red}. When is the entanglement minimised, and maximised? What are the corresponding states of the total system? [5]

Solution 2. (a) (i) Since every particle is in a pure state $|\psi\rangle$, the density operator is given by

$$\begin{aligned}\rho = |\psi\rangle\langle\psi| &= \frac{1}{2}(|\uparrow\rangle + i|\downarrow\rangle)(\langle\uparrow| - i\langle\downarrow|) \\ &= \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| - i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|),\end{aligned}$$

which is represented in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis by the matrix $\rho_1 = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix}$.

(ii) For an equal statistical mixture of $|\uparrow\rangle$ and $|\downarrow\rangle$, the density operator is simply

$$\rho = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| \,,$$

represented by the matrix $\rho_2 = \frac{1}{2}\mathbb{1}$, where $\mathbb{1}$ is the identity.

(iii) For an equal statistical mixture of $|\psi_\pm\rangle \equiv (|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2}$, we have

$$\rho = \frac{1}{2}|\psi_+\rangle\langle\psi_+| + \frac{1}{2}|\psi_-\rangle\langle\psi_-| = \frac{1}{2}|\uparrow\rangle\langle\uparrow| + \frac{1}{2}|\downarrow\rangle\langle\downarrow| \,,$$

which is again represented by $\rho_3 = \frac{1}{2}\mathbb{1}$.

(b) Comparing the three density matrices, one finds that (i) is physically distinct from (ii) and (iii). Situations (ii) and (iii) are physically identical as all measurements would yield the same expectation in both.

Since the pure state $|\psi\rangle$ in (i) is an eigenstate of S_y, one can simply measure S_y to distinguish it from the other two cases.

The expectation is given by $\langle S_y\rangle = \mathrm{Tr}(\rho S_y)$. Using the matrices representing ρ and S_y gives: (i) $\langle S_y\rangle = \hbar/2$, (ii) $\langle S_y\rangle = 0$, and (iii) $\langle S_y\rangle = 0$.

(c) In the $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ basis, the initial state $|\uparrow\downarrow\rangle$ is described by the density matrix

$$\rho(0) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} .$$

Hence, the time-evolved density matrix is given by (with $\theta \equiv Jt/\hbar$)

$$\begin{aligned} \rho(t) &= U(t)\rho(0)U^\dagger(t) \\ &= \begin{pmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & \cos\theta & i\sin\theta & 0 \\ 0 & i\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{i\theta} \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} e^{-i\theta} & 0 & 0 & 0 \\ 0 & \cos\theta & -i\sin\theta & 0 \\ 0 & -i\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & e^{-i\theta} \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \cos^2\theta & -i\sin\theta\cos\theta & 0 \\ 0 & i\sin\theta\cos\theta & \sin^2\theta & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} . \end{aligned}$$

From this expression, one can directly infer that $\rho(t)$ describes a pure state $|\psi(t)\rangle$, i.e., $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$, where

$$|\psi(t)\rangle = \cos\theta|\uparrow\downarrow\rangle + i\sin\theta|\downarrow\uparrow\rangle \,.$$

This is also found by applying the evolution operator $U(t)$ to the initial state $|\uparrow\downarrow\rangle$.

(d) We write $\rho(t)$ in operator form as

$$\rho(t) = \cos^2\theta|\uparrow_1\downarrow_2\rangle\langle\uparrow_1\downarrow_2| + \sin^2\theta|\downarrow_1\uparrow_2\rangle\langle\downarrow_1\uparrow_2| + i\sin\theta\cos\theta(|\downarrow_1\uparrow_2\rangle\langle\uparrow_1\downarrow_2| - |\uparrow_1\downarrow_2\rangle\langle\downarrow_1\uparrow_2|) \,,$$

where the explicit labels 1 and 2 help distinguish the two spins. Tracing over the second spin, one finds the reduced density matrix describing the first,

$$\begin{aligned}\rho_{\text{red}} &= \langle\uparrow_2|\,\rho(t)\,|\uparrow_2\rangle + \langle\downarrow_2|\,\rho(t)\,|\downarrow_2\rangle \\ &= \cos^2\theta|\uparrow_1\rangle\langle\uparrow_1| + \sin^2\theta|\downarrow_1\rangle\langle\downarrow_1| \\ &= \begin{pmatrix}\cos^2\theta & 0 \\ 0 & \sin^2\theta\end{pmatrix} ,\end{aligned}$$

in the $\{|\uparrow_1\rangle, |\downarrow_1\rangle\}$ basis.

(e) The entanglement entropy is given by

$$S_{\text{ent}} = -\text{tr}[\rho_{\text{red}}\log\rho_{\text{red}}] = -\sum\nolimits_i \lambda_i \log\lambda_i \ ,$$

where λ_i are the eigenvalues of ρ_{red}. In our case, these are simply $\cos^2\theta$ and $\sin^2\theta$. Thus,

$$S_{\text{ent}} = -\cos^2\theta\log(\cos^2\theta) - \sin^2\theta\log(\sin^2\theta) \ .$$

Clearly, S_{ent} is nonnegative as $0 \le \cos^2\theta, \sin^2\theta \le 1$. It vanishes when either $\cos\theta$ or $\sin\theta$ equals ± 1, i.e., for $\theta \equiv Jt/\hbar = n\pi/2$, $n = 0, 1, 2, \ldots$.

From (c), we find this minimum corresponds to a product state,

$$|\psi(t)\rangle = \pm|\uparrow\downarrow\rangle \quad \text{or} \quad |\psi(t)\rangle = \pm i|\downarrow\uparrow\rangle \ .$$

The entropy is maximised when $\cos^2\theta = \sin^2\theta = 1/2$, i.e., for $\theta = (2n+1)\pi/4$, $n = 0, 1, 2, \ldots$. This is apparent from symmetry and can be checked explicitly by substituting $\cos^2\theta = x$ and setting $dS_{\text{ent}}/dx = 0$, which gives $x = 1/2$ and $S_{\text{ent}}^{\text{max}} = \log 2$.

From (c), such a situation corresponds to an equal superposition of $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ (a Bell state),

$$|\psi(t)\rangle = \pm\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle \pm i|\downarrow\uparrow\rangle) \ .$$

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3 (a) Consider a particle in a time-dependent harmonic well given by the Hamiltonian

$$H(t) = \frac{p^2}{2M} + \frac{1}{2}M(\omega(t))^2 x^2 \ .$$

Write the instantaneous Hamiltonian $H(t)$ in terms of the ladder operators $a(t)$ and $a^\dagger(t)$, where

$$a(t) = \frac{1}{\sqrt{2}}\left(\frac{x}{\xi(t)} + i\frac{\xi(t)}{\hbar}p\right) \quad \text{and} \quad \xi(t) \equiv \sqrt{\frac{\hbar}{M\omega(t)}} \ , \qquad (*)$$

and state its eigenvalues. (You may directly quote the results.) [4]

(b) The particle is initially in the ground state $|0\rangle$ of $H(t=0)$. The frequency $\omega(t)$ is ramped from ω_0 to $2\omega_0$ over an interval τ, i.e., $\omega(t) = \omega_0(1 + t/\tau)$. Without any calculation, argue what condition τ and ω_0 must satisfy for the ramp to be "slow" or *adiabatic*. What would be the final energy in this case? [4]

(c) By expressing x in terms of a_0 and $a_0^\dagger$, show that $H(t)$ can be written as

$$H(t) = H_0 + \frac{1}{4}\hbar\omega_0\left[\left(\frac{\omega(t)}{\omega_0}\right)^2 - 1\right]\left(a_0 + a_0^\dagger\right)^2 \ ,$$

where H_0 is the Hamiltonian for $t = 0$ and $a_0 \equiv a(0)$. $\left[\textit{Use } (*) \textit{ at } t = 0.\right]$ [4]

(d) Use this expression to find the final energy expectation $\langle H(\tau)\rangle$ for a sudden ramp, where the particle has no time react. Why is this energy different from that in the adiabatic case? $\left[\textit{Note: } a_0|0\rangle = 0 \textit{ and } [a(t), a^\dagger(t)] = 1.\right]$ [5]

(e) At any point during the ramp, the state $|\psi(t)\rangle$ can be written as a superposition of the instantaneous energy eigenstates $|n\rangle_t$,

$$|\psi(t)\rangle = \sum_{n=0}^{\infty} c_n(t)|n\rangle_t \ ,$$

where the states are ordered in increasing energy. Assuming we start from the ground state at $t = 0$, which of the coefficients $c_n(t)$ will always be zero? Use symmetry arguments (no calculation required). [3]

(f) Use the time-dependent Schrödinger equation and the result

$$\frac{d|n\rangle_t}{dt} = \frac{\hbar\omega_0}{2\tau}\sum_{m\neq n}\frac{{}_t\langle m|\left[a(t) + a^\dagger(t)\right]^2|n\rangle_t}{E_n(t) - E_m(t)}|m\rangle_t$$

to write the equation of motion for the coefficients in the form

$$\frac{dc_m(t)}{dt} = A_m(t)c_m(t) + \sum_{n\neq m} B_{mn}(t)c_n(t) \ .$$

You do not need to evaluate inner products. Compare the frequency scales in A_m and B_{mn} to explain how the adiabaticity condition is recovered. [5]

Solution 3. (a) The same transformation was used for the time-independent harmonic oscillator to express the Hamiltonian in terms of ladder operators. Hence, the instantaneous Hamiltonian can be written as

$$H(t) = \left[a^\dagger(t)a(t) + 1/2\right]\hbar\omega(t) ,$$

which has eigenvalues $E_n(t) = (n + 1/2)\hbar\omega(t)$, $n = 0, 1, 2, \ldots$.

(b) For the sweep to be "slow" or adiabatic, the interval τ must be sufficiently large. The only other timescale is $1/\omega_0$, which governs the dynamics of the unperturbed system. Thus, adiabaticity requires $\tau \gg 1/\omega_0$, or $\omega_0\tau \gg 1$.

For an adiabatic sweep, the particle stays in the instantaneous ground state. So the final energy is just the ground state energy of the final Hamiltonian, which is $E_0(\tau) = \hbar\omega_0$.

(c) Adding Eq. $(*)$ and its Hermitian conjugate at $t = 0$, one finds

$$x = \sqrt{\frac{\hbar}{2M\omega_0}}\,\left(a_0 + a_0^\dagger\right) .$$

Using this expression, the instantaneous Hamiltonian can be written as

$$\begin{aligned} H(t) &= \left[\frac{p^2}{2M} + \frac{1}{2}M\omega_0^2 x^2\right] + \frac{1}{2}M\left[(\omega(t))^2 - \omega_0^2\right]x^2 \\ &= H_0 + \frac{1}{2}M\left[(\omega(t))^2 - \omega_0^2\right]\left[\frac{\hbar}{2M\omega_0}\left(a_0 + a_0^\dagger\right)^2\right] \\ &= H_0 + \frac{1}{4}\hbar\omega_0\left[\left(\frac{\omega(t)}{\omega_0}\right)^2 - 1\right]\left(a_0 + a_0^\dagger\right)^2 . \end{aligned}$$

(d) For a sudden ramp, the particle has no time to react, so the final state is the same as the initial state, $|0\rangle$. Hence, the final energy is given by

$$\begin{aligned} \langle 0|H(\tau)|0\rangle &= \langle 0|H_0|0\rangle + \frac{3}{4}\hbar\omega_0\,\langle 0|\left(a_0 + a_0^\dagger\right)^2|0\rangle \\ &= \frac{1}{2}\hbar\omega_0 + \frac{3}{4}\hbar\omega_0\,\langle 0|a_0^2 + a_0^{\dagger 2} + a_0^\dagger a_0 + a_0 a_0^\dagger|0\rangle . \end{aligned}$$

The first three operators in the matrix element give zero, as $a_0|0\rangle = 0 = \langle 0|a_0^\dagger$. The last term is simplified using the commutator $[a_0, a_0^\dagger] = 1$, yielding

$$\begin{aligned} \langle 0|H(\tau)|0\rangle &= \frac{1}{2}\hbar\omega_0 + \frac{3}{4}\hbar\omega_0\,\langle 0|a_0^\dagger a_0 + 1|0\rangle \\ &= \frac{1}{2}\hbar\omega_0 + \frac{3}{4}\hbar\omega_0 = \frac{5}{4}\hbar\omega_0 . \end{aligned}$$

This energy is higher than that in the adiabatic case because the sudden ramp excites transitions to higher energy levels. After the ramp, the particle is no longer in the final ground state, but in a superposition of ground and excited states.

(e)
– The Hamiltonian is always symmetric about the origin ($x = 0$), i.e., has a definite parity. So it cannot couple even and odd wavefunctions, and parity is conserved.
– The particle is initially in the ground state which has an even wavefunction, so it will always have even parity.
– Therefore, the amplitudes of all odd states will be zero, i.e., $c_n(t) = 0$ for $n = 1, 3, 5, \ldots$.

(f) Applying the time-dependent Schrödinger equation to the expansion in terms of the instantaneous eigenstates $|n\rangle_t$, one finds

$$i\hbar \frac{d}{dt} \sum_n c_n(t)|n\rangle_t = H(t) \sum_n c_n(t)|n\rangle_t \; ,$$

$$\text{or} \quad i\hbar \sum_n \left[\frac{dc_n(t)}{dt} |n\rangle_t + c_n(t) \frac{d|n\rangle_t}{dt} \right] = \sum_n E_n(t) c_n(t) |n\rangle_t \; .$$

Taking inner product with ${}_t\langle m|$ and using orthonormality of eigenstates give

$$i\hbar \left[\frac{dc_m(t)}{dt} + \sum_n {}_t\langle m| \frac{d}{dt} |n\rangle_t \, c_n(t) \right] = E_m(t) c_m(t) \; .$$

We then substitute $E_m = (m+1/2)\hbar\omega(t)$ and the expression provided for $d|n\rangle_t/dt$, finding the equations of motion

$$\frac{dc_m(t)}{dt} = A_m(t) c_m(t) + \sum_{n \neq m} B_{mn}(t) c_n(t) \; ,$$

with the coefficients

$$A_m(t) = -i\left(m + \frac{1}{2}\right)\omega(t) \quad \text{and} \quad B_{mn}(t) = \frac{\omega_0}{2\tau\omega(t)} \frac{{}_t\langle m| \left[a(t) + a^\dagger(t)\right]^2 |n\rangle_t}{m-n} \; .$$

Since $\omega(t) \sim \omega_0$, the frequency scales of A_m and B_{mn} are given by ω_0 and $1/\tau$, respectively. Adiabaticity requires $B_{mn} \ll A_m \implies 1/\tau \ll \omega_0$, or $\omega_0\tau \gg 1$, as found in (b).

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4 The Hamiltonian for a set of interacting bosons is $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$ where

$$\begin{aligned} \hat{H}_{\text{kin}} &= -\frac{\hbar^2}{2M}\int d^3\boldsymbol{r}\ \hat{\psi}^\dagger(\boldsymbol{r})\boldsymbol{\nabla}^2\hat{\psi}(\boldsymbol{r})\,, \\ \hat{H}_{\text{int}} &= \frac{1}{2}\int d^3\boldsymbol{r}\int d^3\boldsymbol{r}'\ \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}')U(\boldsymbol{r}-\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r})\,. \end{aligned}$$

and the bosonic field operators, $\hat{\psi}^\dagger(\boldsymbol{r})$ and $\hat{\psi}(\boldsymbol{r})$, satisfy $[\hat{\psi}(\boldsymbol{r}),\hat{\psi}^\dagger(\boldsymbol{r}')] = \delta^3(\boldsymbol{r}-\boldsymbol{r}')$, $[\hat{\psi}(\boldsymbol{r}),\hat{\psi}(\boldsymbol{r}')] = [\hat{\psi}^\dagger(\boldsymbol{r}),\hat{\psi}^\dagger(\boldsymbol{r}')] = 0$.

(a) The plane-waves $\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ provide an orthonormal basis of single-particle states in a system of volume V. Show that the creation and annihilation operators for these states, denoted by $\hat{a}^\dagger_{\boldsymbol{k}}$ and $\hat{a}_{\boldsymbol{k}}$, satisfy $[\hat{a}_{\boldsymbol{k}},\hat{a}^\dagger_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k},\boldsymbol{k}'}$, $[\hat{a}_{\boldsymbol{k}},\hat{a}_{\boldsymbol{k}'}] = [\hat{a}^\dagger_{\boldsymbol{k}},\hat{a}^\dagger_{\boldsymbol{k}'}] = 0$, and that [8]

$$\hat{H}_{\text{kin}} = \sum_{\boldsymbol{k}} \frac{\hbar^2|\boldsymbol{k}|^2}{2M}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}}\,.$$

(b) Show that the interaction energy $\hat{H}_{\text{int}}$ can be written in terms of the density operator $\hat{\rho}(\boldsymbol{r}) \equiv \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})$, by combining both two-body and one-body terms. [4]

(c) Show that the Fourier transform of the density operator, $\hat{\rho}_{\boldsymbol{q}} \equiv \int d^3\boldsymbol{r}\hat{\rho}(\boldsymbol{r})e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}$, may be written [3]

$$\hat{\rho}_{\boldsymbol{q}} = \sum_{\boldsymbol{p}} \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}}\hat{a}_{\boldsymbol{p}}\,.$$

Starting from the exact groundstate, $|\mathrm{GS}\rangle$, approximate descriptions of the low-energy excitations of $\hat{H}$ can be constructed by the variational states

$$|\Psi_{\boldsymbol{q}}\rangle = \frac{1}{\sqrt{S_{\boldsymbol{q}}}}\hat{\rho}_{\boldsymbol{q}}|\mathrm{GS}\rangle\,,$$

with $\hat{\rho}_{\boldsymbol{q}}$ the Fourier transform of the density operator and $S_{\boldsymbol{q}}$ a normalization factor. The variational energy can be shown to be

$$\Delta_{\boldsymbol{q}} = \frac{1}{2S_{\boldsymbol{q}}}\langle\mathrm{GS}|\left[\hat{\rho}^\dagger_{\boldsymbol{q}},\left[\hat{H},\hat{\rho}_{\boldsymbol{q}}\right]\right]|\mathrm{GS}\rangle\,.$$

(d) Show that $|\Psi_{\boldsymbol{q}}\rangle$ is orthogonal to $|\mathrm{GS}\rangle$ for $\boldsymbol{q} \neq 0$, provided $|\mathrm{GS}\rangle$ describes a state of uniform particle density. [2]

(e) Explain why $\left[\hat{H}_{\text{int}},\hat{\rho}_{\boldsymbol{q}}\right] = 0$. Hence show that

$$\left[\hat{H},\hat{\rho}_{\boldsymbol{q}}\right] = -\frac{\hbar^2}{M}\sum_{\boldsymbol{k}} \boldsymbol{k}\cdot\boldsymbol{q}\ \hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2}\hat{a}_{\boldsymbol{k}+\boldsymbol{q}/2}\,.$$

Deduce an expression for the variational energy $\Delta_{\boldsymbol{q}}$. [8]

[*You may use the following identity without proof:*
$[AB,CD] = A[B,C]D + AC[B,D] + [A,C]DB + C[A,D]B$]

Solution 4. (a) Under the change of basis

$$\begin{aligned} a^\dagger_{\boldsymbol{k}} &= \int \phi_{\boldsymbol{k}}(\boldsymbol{r})\psi^\dagger(\boldsymbol{r})d^3\boldsymbol{r} \\ a_{\boldsymbol{k}} &= \int \phi^*_{\boldsymbol{k}}(\boldsymbol{r})\psi(\boldsymbol{r})d^3\boldsymbol{r} \end{aligned}$$

Therefore

$$\begin{aligned} \left[a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}\right] &= \int\int \left[\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')\right] \phi^*_{\boldsymbol{k}}(\boldsymbol{r})\phi_{\boldsymbol{k}'}(\boldsymbol{r}')d^3\boldsymbol{r}d^3\boldsymbol{r}' \\ &= \int \phi^*_{\boldsymbol{k}}(\boldsymbol{r})\phi_{\boldsymbol{k}'}(\boldsymbol{r})d^3\boldsymbol{r} \\ &= \delta_{\boldsymbol{k},\boldsymbol{k}'} \end{aligned}$$

using the fact the states are orthonormal. The cases $\left[a^\dagger_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{k}'}\right] = [a_{\boldsymbol{k}}, a_{\boldsymbol{k}'}] = 0$ follow similarly using the fact that field operators commute.

Inverting the change of basis

$$\begin{aligned} \psi^\dagger(\boldsymbol{r}) &= \sum_{\boldsymbol{k}} \phi^*_{\boldsymbol{k}}(\boldsymbol{r})a^\dagger_{\boldsymbol{k}} \\ \psi(\boldsymbol{r}) &= \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(\boldsymbol{r})a_{\boldsymbol{k}} \end{aligned}$$

gives

$$\begin{aligned} \hat{H}_{\text{kin}} &= -\frac{\hbar^2}{2M}\int d^3\boldsymbol{r} \sum_{\boldsymbol{k},\boldsymbol{k}'} \phi^*_{\boldsymbol{k}}(\boldsymbol{r})a^\dagger_{\boldsymbol{k}}\left[-\boldsymbol{k}'^2\right]\phi_{\boldsymbol{k}'}(\boldsymbol{r})a_{\boldsymbol{k}'} \\ &= -\frac{\hbar^2}{2M}\sum_{\boldsymbol{k},\boldsymbol{k}'}\left[-\boldsymbol{k}'^2\right]a^\dagger_{\boldsymbol{k}}a_{\boldsymbol{k}'}\delta_{\boldsymbol{k},\boldsymbol{k}'} \qquad \text{using orthogonality} \\ &= \sum_{\boldsymbol{k}} \frac{\hbar^2|\boldsymbol{k}|^2}{2M}\hat{a}^\dagger_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}} \end{aligned}$$

(b) The operator appearing inside the integral of H_{int} may be rewritten

$$\begin{aligned} \psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) &= \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}') - \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')\delta(\boldsymbol{r}-\boldsymbol{r}') \\ &= \rho(\boldsymbol{r})\rho(\boldsymbol{r}') - \delta(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}) \end{aligned}$$

(c)

$$\begin{aligned} \hat{\rho}_{\boldsymbol{q}} \equiv \int d^3\boldsymbol{r}\hat{\rho}(\boldsymbol{r})e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} &= \int d^3\boldsymbol{r}\sum_{\boldsymbol{p},\boldsymbol{k}}\phi^*_{\boldsymbol{p}}(\boldsymbol{r})a^\dagger_{\boldsymbol{p}}\phi_{\boldsymbol{k}}(\boldsymbol{r})a_{\boldsymbol{k}}e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \\ &= \frac{1}{V}\int d^3\boldsymbol{r}\sum_{\boldsymbol{p},\boldsymbol{k}}a^\dagger_{\boldsymbol{p}}a_{\boldsymbol{k}}e^{\mathrm{i}(\boldsymbol{k}-\boldsymbol{p}-\boldsymbol{q})\cdot\boldsymbol{r}} \\ &= \sum_{\boldsymbol{p},\boldsymbol{k}}a^\dagger_{\boldsymbol{p}}\delta_{\boldsymbol{k},\boldsymbol{p}+\boldsymbol{q}} = \sum_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k}-\boldsymbol{q}}a_{\boldsymbol{k}} \end{aligned}$$

(d)

$$\begin{aligned}
\langle \mathrm{GS}|\Psi_{\boldsymbol{q}}\rangle \propto \langle \mathrm{GS}|\rho_{\boldsymbol{q}}|\mathrm{GS}\rangle &= \int d^3\boldsymbol{r}\langle \mathrm{GS}|\hat{\rho}(\boldsymbol{r})|\mathrm{GS}\rangle e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \\
\text{But...}\langle \mathrm{GS}|\hat{\rho}(\boldsymbol{r})|\mathrm{GS}\rangle &= \text{Const.} \quad \text{for constant density state} \\
\Rightarrow \int d^3\boldsymbol{r}\langle \mathrm{GS}|\hat{\rho}(\boldsymbol{r})|\mathrm{GS}\rangle e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} &\propto \delta_{\boldsymbol{q},\boldsymbol{0}}
\end{aligned}$$

i.e. the overlap vanishes for $\boldsymbol{q} \neq 0$

(e) We have shown above that $\hat{H}_{\mathrm{int}}$ can be written in terms of $\rho(\boldsymbol{r})$. It therefore must commute with $\rho(\boldsymbol{r})$ and therefore also with $\rho_{\boldsymbol{q}}$

First commutator:

$$\begin{aligned}
[H, \rho_{\boldsymbol{q}}] = [H_{\mathrm{kin}}, \rho_{\boldsymbol{q}}] &= \frac{\hbar^2}{2M}\sum_{\boldsymbol{p},\boldsymbol{k}} k^2 \left[a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}, a^\dagger_{\boldsymbol{p},-\boldsymbol{q}} a_{\boldsymbol{p}}\right] \\
a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} a^\dagger_{\boldsymbol{p},-\boldsymbol{q}} a_{\boldsymbol{p}} - a^\dagger_{\boldsymbol{p},-\boldsymbol{q}} a_{\boldsymbol{p}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} &= \delta_{\boldsymbol{k},\boldsymbol{p}-\boldsymbol{q}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{p}} - \delta_{\boldsymbol{k},\boldsymbol{p}} a^\dagger_{\boldsymbol{p},-\boldsymbol{q}} a_{\boldsymbol{k}} \\
\Rightarrow [H_{\mathrm{kin}}, \rho_{\boldsymbol{q}}] &= \frac{\hbar^2}{2M}\sum_{\boldsymbol{k}} k^2 \left(a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}+\boldsymbol{q}} - a^\dagger_{\boldsymbol{k},-\boldsymbol{q}} a_{\boldsymbol{k}}\right) \\
&= \frac{\hbar^2}{2M}\sum_{\boldsymbol{k}} [|\boldsymbol{k}-\boldsymbol{q}/2|^2 - |\boldsymbol{k}+\boldsymbol{q}/2|^2] a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2} \\
&= -\frac{\hbar^2}{M}\sum_{\boldsymbol{k}} \boldsymbol{k}\cdot\boldsymbol{q}\; a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2}
\end{aligned}$$

Second commutator:

$$\begin{aligned}
\left[\rho^\dagger_{\boldsymbol{q}}, [H_{\mathrm{kin}}, \rho_{\boldsymbol{q}}]\right] &= -\frac{\hbar^2}{M}\sum_{\boldsymbol{p},\boldsymbol{k}} \boldsymbol{k}\cdot\boldsymbol{q}\left[a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p},-\boldsymbol{q}}, a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2}\right] \\
a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p},-\boldsymbol{q}} a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2} - a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2} a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{p},-\boldsymbol{q}} &= a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{k}+\boldsymbol{q}/2}\delta_{\boldsymbol{k}-\boldsymbol{q}/2,\boldsymbol{p}-\boldsymbol{q}} - a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{p},-\boldsymbol{q}}\delta_{\boldsymbol{p},\boldsymbol{k}+\boldsymbol{q}/2} \\
\Rightarrow \left[\rho^\dagger_{\boldsymbol{q}}, [H_{\mathrm{kin}}, \rho_{\boldsymbol{q}}]\right] &= -\frac{\hbar^2}{M}\sum_{\boldsymbol{k},\boldsymbol{p}} \boldsymbol{k}\cdot\boldsymbol{q}\left[a^\dagger_{\boldsymbol{p}} a_{\boldsymbol{k}+\boldsymbol{q}/2}\delta_{\boldsymbol{k}-\boldsymbol{q}/2,\boldsymbol{p}-\boldsymbol{q}} - a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{p},-\boldsymbol{q}}\delta_{\boldsymbol{p},\boldsymbol{k}+\boldsymbol{q}/2}\right] \\
&= -\frac{\hbar^2}{M}\sum_{\boldsymbol{k}} \boldsymbol{k}\cdot\boldsymbol{q}\left[a^\dagger_{\boldsymbol{k}+\boldsymbol{q}/2} a_{\boldsymbol{k}+\boldsymbol{q}/2} - a^\dagger_{\boldsymbol{k}-\boldsymbol{q}/2} a_{\boldsymbol{k}-\boldsymbol{q}/2}\right] \\
&= -\frac{\hbar^2}{M}\sum_{\boldsymbol{k}} \{(\boldsymbol{k}-\boldsymbol{q}/2)\cdot\boldsymbol{q} - (\boldsymbol{k}+\boldsymbol{q}/2)\cdot\boldsymbol{q}\}\, a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}} \\
&= \frac{\hbar^2|\boldsymbol{q}|^2}{M}\sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}
\end{aligned}$$

But $\sum_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k}} a_{\boldsymbol{k}}$ is the total number operator, N. Therefore,

$$\Delta_{\boldsymbol{q}} = \frac{\hbar^2|\boldsymbol{q}|^2}{2M}\frac{N}{S_{\boldsymbol{q}}}$$

END OF PAPER