NATURAL SCIENCES TRIPOS Part II

Wednesday 28 April 2021, 2pm to 4pm

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.

V7.1

A

1 A set of laser fields couple two electronic levels in an atom at position $\boldsymbol{r} = (x, y)$, giving rise to a position-dependent effective potential

$$\mathbb{V}(\boldsymbol{r}) = V_0 \begin{pmatrix} \sinh y & \mathrm{e}^{\mathrm{i}kx} \\ \mathrm{e}^{-\mathrm{i}kx} & -\sinh y \end{pmatrix}$$

expressed here in the basis of the two electronic levels.

Consider first the situation in which the atom is moved at a constant speed v along the line $y = 0$, such that $\boldsymbol{r}(t) = (x, y) = (vt, 0)$.

(a) Determine the instantaneous energies $E_\pm(t)$ and instantaneous eigenstates $|\pm, \boldsymbol{r}(t)\rangle$ for a stationary atom at the position $\boldsymbol{r}(t) = (x, y) = (vt, 0)$. [5]

(b) By expanding the wavefunction as

$$|\Psi(t)\rangle = c_+(t)|+, \boldsymbol{r}(t)\rangle + c_-(t)|-, \boldsymbol{r}(t)\rangle$$

and using the time-dependent Schrödinger equation, show that the electronic state of the atom will evolve adiabatically for $\hbar|\langle -, \boldsymbol{r}(t)|\frac{d}{dt}|+, \boldsymbol{r}(t)\rangle \ll V_0$. Use your results from (a) to deduce the condition on velocity v for which adiabaticity holds. [8]

Now consider the atom to have a mass m, and to move freely in the x, y-plane under the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 \otimes \mathbb{1} + \mathbb{V}(\boldsymbol{r})$$

where $\mathbb{1}$ is the identity operator in the space of the two electronic levels and $\mathbb{V}(\boldsymbol{r})$ is the optical potential described above, whose local eigenstates are $|\pm, \boldsymbol{r}\rangle$.

By expanding the wavefunction as

$$|\Psi(\boldsymbol{r})\rangle = \psi_+(\boldsymbol{r})|+, \boldsymbol{r}\rangle + \psi_-(\boldsymbol{r})|-, \boldsymbol{r}\rangle$$

and *making the adiabatic assumption*, the time-independent Schrödinger equation, $H|\Psi(\boldsymbol{r})\rangle = E|\Psi(\boldsymbol{r})\rangle$ can be written as the two equations

$$\langle \pm, \boldsymbol{r}| \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \mathbb{V}(\boldsymbol{r})\right] \psi_\pm(\boldsymbol{r})|\pm, \boldsymbol{r}\rangle = E\psi_\pm(\boldsymbol{r}) \qquad (\star)$$

for the wavefunctions $\psi_\pm(\boldsymbol{r})$ describing atoms in the two energy levels.

(c) Show that the equations $(\star)$ lead to effective Hamiltonians $H_\pm\psi_\pm(\boldsymbol{r}) = E\psi_\pm(\boldsymbol{r})$, with

$$H_\pm = \frac{1}{2m}\left(\frac{\hbar}{\mathrm{i}}\boldsymbol{\nabla} + \hbar\boldsymbol{A}_\pm\right)^2 + V_\pm(\boldsymbol{r})$$

where $\boldsymbol{A}_\pm(\boldsymbol{r}) = -\mathrm{i}\langle \pm, \boldsymbol{r}|\boldsymbol{\nabla}|\pm, \boldsymbol{r}\rangle$. Deduce a general expression for $V_\pm(\boldsymbol{r})$. [8]

(d) Outline the conditions under which the adiabaticity assumption leading to $(\star)$ holds. [4]

Solution 1. (a) On the line $y = 0$

$$\mathbb{V}(x, y=0) = V_0 \begin{pmatrix} 0 & \mathrm{e}^{\mathrm{i}kx} \\ \mathrm{e}^{-\mathrm{i}kx} & 0 \end{pmatrix}$$

The energies are $E_\pm(x) = \pm V_0$ and the states are

$$|\pm, x(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm\mathrm{e}^{-\mathrm{i}kx} \end{pmatrix}$$

(b)

$$\mathrm{i}\hbar|\dot{\psi}\rangle = \mathbb{V}|\psi\rangle$$

$$\begin{aligned} i\hbar\dot{c}_+|+,t\rangle + i\hbar c_+\frac{d}{dt}|+,t\rangle &= E_+c_+|+,t\rangle \\ i\hbar\dot{c}_-|-,t\rangle + i\hbar c_-\frac{d}{dt}|-,t\rangle &= E_-c_-|-,t\rangle \end{aligned}$$

Taking $\langle\pm, t|$ on these gives

$$\begin{aligned} i\hbar\dot{c}_+ &= E_+c_+ - i\hbar c_+\langle +,t|\frac{d}{dt}|+,t\rangle - i\hbar c_-\langle +,t|\frac{d}{dt}|-,t\rangle \\ i\hbar\dot{c}_- &= E_-c_- - i\hbar c_-\langle -,t|\frac{d}{dt}|-,t\rangle - i\hbar c_+\langle -,t|\frac{d}{dt}|+,t\rangle \end{aligned}$$

Adiabatic provided the off-diagonal parts are negligible

$$\hbar|\langle +, x(t)|\frac{d}{dt}|-, x(t)\rangle| \ll (E_+ - E_-)/2 = V_0$$

Use $|-, x(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{e}^{-\mathrm{i}kvt} \end{pmatrix}$ to compute

$$\frac{d}{dt}|-, x(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ +ikv\mathrm{e}^{-\mathrm{i}kvt} \end{pmatrix}$$

from which $< +, x|(d/dt)|-, x\rangle = ikv/2$.

Thus we need $\hbar vk/2 \ll V_0$, i.e.

$$v \ll \frac{V_0}{2\hbar k}$$

(c)

$$\langle\pm| \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right] \psi_\pm|\pm\rangle = E\psi_\pm$$

Expand out

$$\begin{aligned} \langle\pm|\nabla^2\psi_\pm|\pm\rangle &= \langle\pm|\nabla\cdot[(\nabla\psi_\pm)|\pm\rangle + \psi_\pm\nabla|\pm\rangle] \\ &= \langle\pm|\pm\rangle\nabla^2\psi_\pm + 2\langle\pm|\nabla|\pm\rangle\cdot\nabla\psi_\pm + \psi_\pm\langle\pm|\nabla^2|\pm\rangle \end{aligned}$$

Define $A_\pm \equiv -\mathrm{i}\langle\pm|\nabla|\pm\rangle$ to write

$$\begin{aligned}
\frac{1}{2m}\left[-\hbar^2\nabla^2\psi_\pm + \frac{2\hbar^2}{i}\nabla\psi_\pm\cdot A_\pm - \hbar^2\langle\pm|\nabla^2|\pm\rangle\psi_\pm\right] &= E_\pm\psi_\pm \\
\frac{1}{2m}\left[\left(\frac{\hbar}{i}+\hbar A_\pm\right)^2 - \hbar^2|A_\pm|^2 - \hbar^2\langle\pm|\nabla^2|\pm\rangle\right]\psi_\pm &= E_\pm\psi_\pm \\
\Rightarrow H_\pm\psi_\pm &= E_\pm\psi_\pm \\
\text{with} H_\pm &= \frac{1}{2m}\left(\frac{\hbar}{i}\nabla+\hbar A_\pm\right)^2 + V_\pm \\
V_\pm(r) &= E_\pm(r) - \frac{\hbar^2}{2m}\left(|A_\pm|^2 + \langle\pm|\nabla^2|\pm\rangle\psi_\pm\right)
\end{aligned}$$

(d) We require that the off-diagonal elements are small compared to the energy spacing of adiabatic levels. Credit will be given for this statement, and reasoned cases setting the effective size of the off-diagonal elements.

This requires:

- $\left|\frac{\hbar^2}{2m}\langle -,\boldsymbol{r}|\nabla^2|+,\boldsymbol{r}\rangle\right| \ll |E_+ - E_-|$
- $\left|\frac{\hbar^2}{2m}\psi_+^*\nabla\psi_+\cdot A_{-+}\right| \ll |E_+ - E_-||\psi_+|^2$ where $A_{-+} \equiv -i\langle -,\boldsymbol{r}|\boldsymbol{\nabla}|+,\boldsymbol{r}\rangle$

The second condition is essentially equivalent to the condition in (b)

$$|\hbar\langle -,\boldsymbol{r}(t)|\frac{d}{dt}| + \boldsymbol{r}(t)\rangle| \ll |E_+ - E_-|$$

with the instantaneous velocity $\dot{\boldsymbol{r}}(t)$ denoting the local velocity $\frac{\hbar}{m}|\psi_+^*\nabla\psi_+|/|\psi_+|^2$

2 The propagator for a quantum particle moving in one dimension is defined as

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

where $|x\rangle$ are the position eigenstates, $U(t,t')$ is the time-evolution operator from initial time t' to final time t, and $\theta(t)$ is the Heaviside step function.

(a) Show that, for a Hamiltonian $H(t) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x,t)$, the propagator satisfies

$$\left[\mathrm{i}\hbar\frac{\partial}{\partial t} - H(t)\right] K(x,t|x',t') = \mathrm{i}\hbar\delta(t-t')\delta(x-x')$$

with the boundary condition that $K(x,t|x',t') = 0$ for $t < t'$. [5]

For a simple harmonic oscillator, with Hamiltonian $H_0 = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2$, the propagator starting from $x' = 0$ at $t' = 0$ is

$$K_0(x,t|0,0) = \theta(t)\sqrt{\frac{m\omega}{2\pi\mathrm{i}\hbar\sin\omega t}}\exp\left(\mathrm{i}\frac{m\omega}{2\hbar}x^2\cot\omega t\right) .$$

(b) Show that, in the presence of a time-dependent force, $H = H_0 - xF(t)$, the solution to the equation in part (a) can be found, for $x' = t' = 0$, by writing

$$K(x,t|0,0) = K_0(x,t|0,0)\exp\left[\mathrm{i}G(x,t)/\hbar\right]$$

with $G(x,t) = A(t) + B(t)x$, provided that

$$\begin{aligned} \dot{A}(t) &= -\frac{B(t)^2}{2m} \\ \dot{B}(t) + \omega\cot(\omega t)B(t) &= F(t). \end{aligned}$$

Hence, find an expression for $B(t)$. [12]
[*Hint: multiply the differential equation by* $\sin\omega t$.]

(c) By making reference to the Feynman path integral formulation of quantum mechanics, comment on the relation of these results to the classical trajectory. [8]

Solution 2. (a) Note that the Heaviside function corresponds the boundary condition. Inserting the expression for the propagator to the Schrödinger equation gives

$$\begin{aligned}\left[\mathrm{i}\hbar\frac{\partial}{\partial t}-H(t)\right]\theta(t-t')\langle x|U(t,t')|x'\rangle &= \mathrm{i}\hbar\delta(t-t')\langle x|U(t,t')|x'\rangle \\ &\quad +\mathrm{i}\hbar\theta(t-t')\langle x|\frac{\partial U(t,t')}{\partial t}|x'\rangle-\theta(t-t')H(t)\langle x|U(t,t')|x'\rangle,\end{aligned}$$

upon employing $\partial_t\theta(t-t')=\delta(t-t')$. The terms involving the Heaviside function cancels when we use the fact that $\partial_t U=-\frac{\mathrm{i}}{\hbar}HU$. This gives

$$\begin{aligned}\left[\mathrm{i}\hbar\frac{\partial}{\partial t}-H(t)\right]\theta(t-t')\langle x|U(t,t')|x'\rangle &= \mathrm{i}\hbar\delta(t-t')\langle x|U(t,t')|x'\rangle \\ &= \mathrm{i}\hbar\delta(t-t')\langle x|x'\rangle=\mathrm{i}\hbar\delta(t-t')\delta(x-x')\end{aligned}$$

(b) For the simple harmonic oscillator, we have

$$\left[\mathrm{i}\hbar\frac{\partial}{\partial t}-H_0\right]K_0(x,t|0,0)=\mathrm{i}\hbar\delta(t)\delta(x),$$

which corresponds to the Schrödinger equation for $t>0$.

So, for the driven harmonic oscillator:

$$\begin{aligned}\left[\mathrm{i}\hbar\frac{\partial}{\partial t}-H_0+xF(t)\right]K_0e^{\mathrm{i}G/\hbar} &= \underbrace{\left[\mathrm{i}\hbar\frac{\partial K_0}{\partial t}-H_0K_0\right]}_{0}e^{\mathrm{i}G/\hbar}-K_0\frac{\partial G}{\partial t}e^{\mathrm{i}G/\hbar} \\ &\quad +\frac{\hbar^2}{2m}\left[\frac{2i}{\hbar}\frac{\partial K_0}{\partial x}\frac{\partial G}{\partial x}-\frac{K_0}{\hbar^2}\left(\frac{\partial G}{\partial x}\right)^2\right]e^{\mathrm{i}G/\hbar} \\ 0 &= -\frac{\partial G}{\partial t}-\omega x\cot(\omega t)\frac{\partial G}{\partial x}-\frac{1}{2m}\left(\frac{\partial G}{\partial x}\right)^2+F(t)x\end{aligned}$$

where, on the last line, we used

$$\frac{\partial K_0}{\partial x}=K_0\frac{\mathrm{i}m\omega}{\hbar}x\cot(\omega t).$$

For $G(x,t)=A(t)+B(t)x$, this gives

$$-\dot{A}-\dot{B}x-\omega x\cot(\omega x)B-\frac{1}{2m}B^2+Fx=0\,.$$

Equating terms for each power of x:

$$\begin{aligned}\dot{A}(t) &= -\frac{B(t)^2}{2m} \\ \dot{B}(t)+\omega\cot(\omega t)B(t) &= F(t).\end{aligned}$$

Modifying the second line:

$$\begin{aligned} \dot{B}\sin(\omega t) + \omega\cos(\omega t)B(t) &= F(t)\sin(\omega t) \\ \frac{\mathrm{d}}{\mathrm{d}t}\left[B\sin(\omega t)\right] &= F(t)\sin(\omega t) \\ B(t) &= \frac{1}{\sin(\omega t)}\int_0^t \mathrm{d}t' F(t')\sin(\omega t'). \end{aligned}$$

(c) The path integral formulation expresses the propagator as the sum over all paths, $x(t)$, weighted by $e^{iS[x(t)]/\hbar}$ with S the action, and with $x(t)$ satisfying the boundary conditions $x(t_i)$ and $x(t_f)$ at initial and final times, t_i and t_f,

$$K \sim \int_{x(t_i)\to x(t_f)} \mathcal{D}x(t)e^{iS[x(t)]/\hbar}$$

Since for the (driven) harmonic oscillator the action is at most quadratic in $x(t)$ and $\dot{x}(t)$, by expanding $x(t) = x_{cl}(t) + \delta x(t)$ around the classical trajectory $x_c(t)$ – which extremizes the action – this can be written exactly as

$$K \sim e^{iS[x_{cl}(t)]/\hbar}\int_{0\to 0} \mathcal{D}\delta x(t)e^{iS[\delta x(t)]/\hbar}$$

where the remaining path integral of $\delta x(t)$ is independent of the initial and final positions.

Thus, the dependence on $x(t_i)$ and $x(t_f)$ enters only through the prefactor $e^{iS[x_{cl}(t)]/\hbar}$ which is the classical action, determined on the classical trajectory.

The solution here is of this form: the content of the exponent is this classical action.

3 A system of N bosons is described by the second-quantized Hamiltonian

$$H = \int \mathrm{d}\boldsymbol{r}\ \psi^\dagger(\boldsymbol{r})\Big[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V_1(\boldsymbol{r})\Big]\psi(\boldsymbol{r}) + \frac{1}{2}\iint \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\psi^\dagger(\boldsymbol{r})\,\psi^\dagger(\boldsymbol{r}')V_2(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r})$$

where $\psi(\boldsymbol{r})$ and $\psi^\dagger(\boldsymbol{r})$ are the field operators, and $V_2(\boldsymbol{r},\boldsymbol{r}')$ is the two-body interaction potential.

(a) State the set of commutation relations that the field operators satisfy. [3]

(b) Hence show that

$$\left[\psi(\boldsymbol{r}), \int \mathrm{d}\boldsymbol{r}' \left(\frac{\partial}{\partial \boldsymbol{r}'}\psi^\dagger(\boldsymbol{r}')\right) F(\boldsymbol{r}')\right] = -\boldsymbol{\nabla} F(\boldsymbol{r})$$

where $F(\boldsymbol{r})$ commutes with $\psi(\boldsymbol{r})$ and vanishes at large $|\boldsymbol{r}|$. [2]

(c) Write down a second-quantized form for the total momentum operator, $\boldsymbol{P}$. By employing appropriate commutation relations, and assuming that $\psi(\boldsymbol{r})$ and $\psi^\dagger(\boldsymbol{r})$ vanish at large $|\boldsymbol{r}|$, show that the total momentum $\boldsymbol{P}$ is conserved when $V_1 = 0$ and $V_2(\boldsymbol{r},\boldsymbol{r}') = V_2(|\boldsymbol{r}-\boldsymbol{r}'|)$. [8]

[*You may use the facts that* $[AB,C] = A[B,C] + [A,C]B$; $[A,BC] = B[A,C] + [A,B]C$; *and* $\mathrm{d}|\boldsymbol{r}|/\mathrm{d}\boldsymbol{r} = \boldsymbol{r}/|\boldsymbol{r}|$.]

(d) Defining the current density operator as

$$\boldsymbol{J}(\boldsymbol{r}) = \frac{\hbar}{2mi}\Big\{\psi^\dagger(\boldsymbol{r})\boldsymbol{\nabla}\psi(\boldsymbol{r}) - [\boldsymbol{\nabla}\psi^\dagger(\boldsymbol{r})]\psi(\boldsymbol{r})\Big\},$$

show that the particle density $\rho(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$ satisfies the continuity equation

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{J} = 0,$$

in the Heisenberg picture. [8]

(e) How would each of the above answers be affected if the particles were fermions instead of bosons? [4]

Solution 3. (a)

$$[\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')] = \delta(\boldsymbol{r} - \boldsymbol{r}')$$
$$[\psi(\boldsymbol{r}), \psi(\boldsymbol{r}')] = 0$$
$$[\psi^\dagger(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')] = 0$$

(b) Integrate by parts:

$$\begin{aligned}
\int \mathrm{d}\boldsymbol{r}' \left(\boldsymbol{\nabla}_{\boldsymbol{r}'}\psi^\dagger(\boldsymbol{r}')\right) F(\boldsymbol{r}') &= -\int \mathrm{d}\boldsymbol{r}'\psi^\dagger(\boldsymbol{r}')\boldsymbol{\nabla}_{\boldsymbol{r}'}F(\boldsymbol{r}') \\
\left[\psi(\boldsymbol{r}), \int \mathrm{d}\boldsymbol{r}' \left(\boldsymbol{\nabla}_{\boldsymbol{r}'}\psi^\dagger(\boldsymbol{r}')\right) F(\boldsymbol{r}')\right] &= -\int \mathrm{d}\boldsymbol{r}' \left[\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')\right] \boldsymbol{\nabla}_{\boldsymbol{r}}F(\boldsymbol{r}) \\
&= -\boldsymbol{\nabla}_{\boldsymbol{r}}F(\boldsymbol{r})
\end{aligned}$$

(c) Momentum operator is $\boldsymbol{P} = -\mathrm{i}\hbar \int \mathrm{d}\boldsymbol{r}\psi^\dagger(\boldsymbol{r})\boldsymbol{\nabla}\psi(\boldsymbol{r})$.

$$\begin{aligned}
\frac{d\boldsymbol{P}}{dt} &= \frac{\mathrm{i}}{\hbar}[H, \boldsymbol{P}] \\
&= \frac{\hbar^2}{2m}\underbrace{\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}' \left[\boldsymbol{\nabla}_r\psi^\dagger(\boldsymbol{r})\cdot\boldsymbol{\nabla}_r\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')\boldsymbol{\nabla}_{r'}\psi(\boldsymbol{r}')\right]}_{\diamondsuit} \\
&\quad + \underbrace{\frac{1}{2}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{r}'' \left[\psi^\dagger(\boldsymbol{r})\,\psi^\dagger(\boldsymbol{r}')V_2(|\boldsymbol{r}-\boldsymbol{r}'|)\psi(\boldsymbol{r}')\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}'')\boldsymbol{\nabla}_{r''}\psi(\boldsymbol{r}'')\right]}_{\square}
\end{aligned}$$

First commutator gives zero upon using integration by parts where the boundary terms vanish:

$$\begin{aligned}
\diamondsuit &= -\int\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\left[\psi(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')\boldsymbol{\nabla}_{r'}\psi(\boldsymbol{r}')\right] + \left[\psi^\dagger(\boldsymbol{r}), \psi^\dagger(\boldsymbol{r}')\boldsymbol{\nabla}_{r'}\psi(\boldsymbol{r}')\right]\boldsymbol{\nabla}_r^2\psi(\boldsymbol{r}) \\
&= -\int\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\delta(\boldsymbol{r}-\boldsymbol{r}')\left\{\boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\cdot\boldsymbol{\nabla}_{r'}\psi(\boldsymbol{r}') + \boldsymbol{\nabla}_{r'}\psi^\dagger(\boldsymbol{r}')\cdot\boldsymbol{\nabla}_r^2\psi(\boldsymbol{r})\right\} \\
&= -\int \mathrm{d}\boldsymbol{r}\left\{\boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\cdot\boldsymbol{\nabla}_r\psi(\boldsymbol{r}) - \boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\cdot\boldsymbol{\nabla}_r\psi(\boldsymbol{r})\right\} = 0.
\end{aligned}$$

Similarly, the second commutator reduces to

$$\square \propto \int\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'V_2'(|\boldsymbol{r}-\boldsymbol{r}'|)\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}\cdots$$

where both $V_2(|\boldsymbol{r}-\boldsymbol{r}'|)$ and its derivative $V_2'(|\boldsymbol{r}-\boldsymbol{r}'|)$ are symmetric functions, while $\frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}$ changes sign upon changing $\boldsymbol{r}$ and $\boldsymbol{r}'$. Therefore, the integral vanishes and the total momentum is conserved

$$\frac{d\boldsymbol{P}}{dt} = 0$$

(d) Following the algebra in part (c) but for $\rho(\boldsymbol{r}) = \psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r})$:

$$\begin{aligned}
\frac{d\rho(\boldsymbol{r})}{dt} &= \frac{\mathrm{i}}{\hbar}[H,\rho] \\
&= \frac{\mathrm{i}}{\hbar}\frac{\hbar^2}{2m}\int \mathrm{d}\boldsymbol{r}\left[\boldsymbol{\nabla}_r\psi^\dagger(\boldsymbol{r})\cdot\boldsymbol{\nabla}_r\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\right] \\
&\quad +\frac{\mathrm{i}}{\hbar}\int \mathrm{d}\boldsymbol{r}V_1(r)[\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')] \\
&\quad +\frac{\mathrm{i}}{\hbar}\frac{1}{2}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'V_2(\boldsymbol{r},\boldsymbol{r}')\left[\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r}'')\psi(\boldsymbol{r}'')\right]
\end{aligned}$$

The one-body interaction term vanishes as density at two different points commute upon integration:

$$\frac{\mathrm{i}}{\hbar}\int \mathrm{d}\boldsymbol{r}V_1(r)\delta(\boldsymbol{r}-\boldsymbol{r}')\left\{\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}') - \psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})\right\} = 0$$

Similarly, the two-body interaction term vanishes:

$$\begin{aligned}
\ldots &= \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'V_2\left\{\psi^\dagger(\boldsymbol{r}'')\left[\psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}'),\psi(\boldsymbol{r}'')\right]\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) + \psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\left[\psi(\boldsymbol{r}')\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r}'')\right]\psi(\boldsymbol{r}'')\right\} \\
&= \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'V_2\delta(\boldsymbol{r}'-\boldsymbol{r}'')\left\{-\psi^\dagger(\boldsymbol{r}'')\psi^\dagger(\boldsymbol{r})\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) + \psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r})\psi(\boldsymbol{r}'')\right\} \\
&\quad + \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'V_2\delta(\boldsymbol{r}-\boldsymbol{r}'')\left\{-\psi^\dagger(\boldsymbol{r}'')\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) + \psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}')\psi(\boldsymbol{r}')\psi(\boldsymbol{r}'')\right\} \\
&= 0.
\end{aligned}$$

What is left is the continuity equation:

$$\begin{aligned}
\frac{d\rho}{dt} &= -\frac{\mathrm{i}}{\hbar}\frac{\hbar^2}{2m}\int \mathrm{d}\boldsymbol{r}\delta(\boldsymbol{r}-\boldsymbol{r}')\left\{\boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\cdot\psi(\boldsymbol{r}') - \psi^\dagger(\boldsymbol{r}')\boldsymbol{\nabla}_r^2\psi(\boldsymbol{r})\right\} \\
&= \frac{\hbar}{2m\mathrm{i}}\left[\boldsymbol{\nabla}_r^2\psi^\dagger(\boldsymbol{r})\cdot\psi(\boldsymbol{r}) - \psi^\dagger(\boldsymbol{r})\boldsymbol{\nabla}_r^2\psi(\boldsymbol{r})\right] \\
&= -\boldsymbol{\nabla}_r\cdot\boldsymbol{J}.
\end{aligned}$$

(e) They would not change except for (a) where for fermions:

$$\{\psi(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r})\} = \delta(\boldsymbol{r}-\boldsymbol{r}')$$

$$\{\psi(\boldsymbol{r}),\psi(\boldsymbol{r})\} = 0$$

$$\{\psi^\dagger(\boldsymbol{r}),\psi^\dagger(\boldsymbol{r})\} = 0$$

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4 The equation of motion for the density operator of a quantum system is

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \frac{\mathrm{i}}{\hbar}\left[\rho(t), H\right] + \gamma\mathcal{L}[\rho(t)]$$

where H is the Hamiltonian and

$$\mathcal{L}[\rho] \equiv L\rho L^{\dagger} - \frac{1}{2}\left(L^{\dagger}L\rho + \rho L^{\dagger}L\right)$$

describes dissipative coupling to an external environment via some operator L.

(a) Show that the above equation of motion for $\rho(t)$ leaves $\mathrm{Tr}[\rho(t)]$ time-independent. [4]

[*You may use the fact that* $Tr[AB] = Tr[BA]$.]

(b) Show that for a two-level quantum system one can parameterise $\rho(t)$ in terms of three quantities $\rho_{i=x,y,z}(t)$ as

$$\rho(t) = \frac{1}{2}\mathbb{1} + \sum_{i=x,y,z} \rho_i(t)\sigma_i\,,$$

where $\mathbb{1}$ is the 2×2 identity matrix and $\sigma_{x,y,z}$ are the Pauli matrices. [4]

[*The Pauli matrices are* $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.]

Consider a two-level system, with Hamiltonian $H = \hbar\Delta\sigma_z$ and dissipator $L = \sigma_-$, where $\sigma_\pm \equiv \sigma_x \pm \mathrm{i}\sigma_y$.

(c) Show that the equation of motion for $\rho_z(t)$ is [8]

$$\dot{\rho}_z = -4\gamma\rho_z - 2\gamma\,.$$

[*You may use:* $[\sigma_l, \sigma_m] = 2\mathrm{i}\epsilon_{lmn}\sigma_n$, $\sigma_+\sigma_- = 2(\mathbb{1} + \sigma_z), \sigma_-\sigma_+ = 2(\mathbb{1} - \sigma_z)$, *and* $\sigma_-\sigma_x\sigma_+ = \sigma_-\sigma_y\sigma_+ = 0$, $\sigma_-\sigma_z\sigma_+ = 2(\mathbb{1} - \sigma_z)$.]

(d) Given that the remaining equations of motion are $\dot{\rho}_x = -2\Delta\rho_y - 2\gamma\rho_x$ and $\dot{\rho}_y = 2\Delta\rho_x - 2\gamma\rho_y$, determine the steady state density operator to which the system evolves at long times, $t \to \infty$. How is it related to the eigenstates of the Hamiltonian? [4]

The equation of motion is extended to include a second dissipator, as

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \frac{\mathrm{i}}{\hbar}\left[\rho, H\right] + \gamma\mathcal{L}[\rho] + \gamma'\mathcal{L}'[\rho]$$

with $\mathcal{L}'[\rho]$ of the same form as $\mathcal{L}[\rho]$ but with $L = \sigma_-$ replaced by $L' = \sigma_+ \equiv \sigma_x + \mathrm{i}\sigma_-$.

(e) For what value of γ'/γ does the steady state density operator, at $t \to \infty$, describe thermal equilibrium at temperature T? [5]

[*You may use:* $\sigma_-\sigma_x\sigma_+ = \sigma_+\sigma_y\sigma_- = 0$, $\sigma_+\sigma_z\sigma_- = -2(\mathbb{1} + \sigma_z)$.]

Solution 4. (a)

$$\begin{aligned}\frac{d}{dt}\mathrm{Tr}[\rho] &= \frac{\mathrm{i}}{\hbar}\mathrm{Tr}[\rho H - H\rho] + \gamma\mathrm{Tr}[L\rho L^\dagger - (1/2)(L^\dagger L\rho + \rho L^\dagger L)] \\ &= \frac{i}{\hbar}\mathrm{Tr}[\rho H - \rho H] + \gamma\mathrm{Tr}[L^\dagger L\rho - (1/2)(L^\dagger L\rho + L^\dagger L\rho)] \\ &= 0\end{aligned}$$

using cyclic permutation of operators within the trace.

(b) We use the facts that: ρ is a 2×2 matrix; ρ is hermitian; its trace is 1. This leaves only three real parameters that are free to be chosen

$$\rho = \begin{pmatrix} 1/2+\rho_z & \rho_x - \mathrm{i}\rho_y \\ \rho_x + \mathrm{i}\rho_y & 1/2-\rho_z \end{pmatrix}$$

Equivalently, the three Pauli matrix exhaust the traceless 2×2 Hermitian matrices.

(c) We use $L = \sigma_-$ and $L^\dagger = \sigma_+$ to get the full equation of motion

$$\begin{aligned}\dot\rho_i\sigma_i &= \mathrm{i}\mathit{\Delta}[\sigma_i,\sigma_z] + \frac{1}{2}\gamma\sigma_-\sigma_+ - \frac{1}{4}\gamma(2\sigma_+\sigma_-) \\ &\quad +\gamma\rho_i\sigma_-\sigma_i\sigma_+ - \frac{\gamma}{2}\rho_i(\sigma_+\sigma_-\sigma_i + \sigma_i\sigma_+\sigma_-) \\ &= \mathrm{i}\mathit{\Delta}[\sigma_i,\sigma_z] - 2\gamma\sigma_z \\ &\quad +\gamma\rho_i\sigma_-\sigma_i\sigma_+ - \frac{\gamma}{2}\rho_i(\sigma_+\sigma_-\sigma_i + \sigma_i\sigma_+\sigma_-)\end{aligned}$$

where we have used $\sigma_+\sigma_- = 2(1+\sigma_z)$ and $\sigma_-\sigma_+ = 2(1-\sigma_z)$ from the hints.

Now, using $\sigma_-\sigma_x\sigma_+ = \sigma_-\sigma_y\sigma_+ = 0$ and $\sigma_-\sigma_z\sigma_+ = 2(1-\sigma_z)$ we find that the equation of motion for the coefficient of σ_z depends on only ρ_z, i.e.

$$\begin{aligned}\dot\rho_z\sigma_z &= 0 - 2\gamma\sigma_z \\ &\quad +\gamma\rho_z(2(1-\sigma_z) - 2(1+\sigma_z)\sigma_z) \\ &= -2\gamma\sigma_z + \gamma\rho_z(2 - 2\sigma_z - 2\sigma_z - 2)\end{aligned}$$

Note that there are no contributions from the time derivatives of $\rho_x\sigma_x$ and $\rho_y\sigma_z$. Hence, equating the coefficient of σ_z we get

$$\dot\rho_z = -4\gamma\rho_z - 2\gamma\,.$$

(d) Given the other equations, we see that there are steady states with $\rho_x = \rho_y = 0$ and $-2\gamma - 4\gamma\rho_z = 0$, i.e. $\rho_z = -1/2$. Hence [4]

$$\rho(t\to\infty) = 1/2 - 1/2\sigma_z = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

This is a *pure state*. It corresponds to the energy eigenscate of the Hamiltonian with energy $-\hbar\Delta$. Thus for $\Delta > 0$ this is the groundstate. For $\Delta < 0$ it is the excited state.

(e) Adapting the previous derivation, now for γ' and L' leads to an additional term in $\dot{\rho}_z\sigma_z$:

$$\begin{aligned} &+\gamma'\sigma_z + \gamma'\rho_z(\sigma_+\sigma_z\sigma_- - (1/2)\{\sigma_-\sigma_+\sigma_z\}_+ \\ &= +2\gamma'\sigma_z + \gamma'\rho_z(-2(1+\sigma_z) - 2\sigma_z(1-\sigma_z)) \\ &= 2\gamma'\sigma_z - 4\gamma'\rho_z\sigma_z \end{aligned}$$

Hence the new equation of motion is

$$\dot{\rho}_z = -4\gamma\rho_z - 2\gamma - 4\gamma'\rho_z + 2\gamma' \,.$$

The new steady state is

$$\rho_z = \frac{1}{2}\left(\frac{\gamma' - \gamma}{\gamma' + \gamma}\right)$$

which leads to

$$\rho(t \to \infty) = 1/2 + \rho_z\sigma_z = \frac{1}{\gamma + \gamma'}\begin{pmatrix} \gamma' & 0 \\ 0 & \gamma \end{pmatrix}$$

At thermal equilibrium

$$\rho = e^{-\beta H}/Z = \frac{1}{Z}\begin{pmatrix} e^{-\beta\hbar\Delta} & 0 \\ 0 & e^{+\beta\hbar\Delta} \end{pmatrix} ,$$

so $e^{+2\beta\hbar\Delta} = \gamma'/\gamma$. Thus

$$\gamma'/\gamma = e^{-2\hbar\Delta/k_{\mathrm{B}}T} \,.$$
