Quantum Mechanics III

Final Exam

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1. Consider a two-dimensional Hilbert space spanned by the orthogonal vectors $|0\rangle$ and $|1\rangle$. Except for trivial transformations, the two most general vectors in this space with the angle θ between them can always be picked in the form $|\theta^{\pm}\rangle = \cos(\theta/2)|0\rangle \pm \sin(\theta/2)|1\rangle$; for simplicity, choose $0 \leq \theta \leq \pi/2$. For some quantum cryptography reasons, Alice sends one of these two states to Bob, each with probability $1/2$, so that the present problem treats the states $|\theta^{\pm}\rangle$ equally; we are implicitly taking this into account below. Bob then tries to determine which of the two states it was. Also define the states $|\theta_{\perp}^{\pm}\rangle$, unique up to trivial transformations, that are orthogonal to the respective states $|\theta^{\pm}\rangle$.

Now, for any $0 \leq \alpha \leq 1$, $E_{\pm} = \alpha|\theta_{\perp}^{\mp}\rangle\langle\theta_{\perp}^{\mp}|$ are positive operators that qualify as members of a POVM and would then have the property that Bob's measurement with the outcomes "$\pm$" corresponding to the effects $E_{\pm}$ gives an affirmative result only if Alice sent the states $|\theta^{\pm}\rangle$; such a result never misidentifies the state. However, E_{+} and E_{-} alone do not necessarily make a POVM. In general, there has to be a third measurement outcome "0" such that the probability for it is determined by some effect E_0. If there are several outcomes besides "+" and "−", they can always be lumped into such a "0".

(a) Show that $E_0 = 0$ only if $\alpha = 1$ and $\theta = \pi/2$, and $E_0 > 0$ only if $\alpha \leq 1/(1 + \cos\theta)$.

(b) Show that if $E_0 \neq 0$, neither $P_+ = \langle\theta^+|E_0|\theta^+\rangle$, nor $P_- = \langle\theta^-|E_0|\theta^-\rangle$ can be equal to zero. One implication is that if $\theta < \pi/2$, there must be a measurement outcome that does not distinguish between the incoming states $|\theta^+\rangle$ and $|\theta^-\rangle$.

(c) Show that for a given angle θ, the smallest possibly probability for an ambiguous result is $\cos\theta$.

(a) Let us define the orthogonal vectors to $|\theta^{\pm}\rangle$ as

$$|\theta_{\perp}^{\pm}\rangle = \mp\sin(\theta/2)\,|0\rangle + \cos(\theta/2)\,|1\rangle.$$

These are unique up to a trivial transformation. Now, as a POVM

$$\sum_k E_k = \alpha E_+ + \alpha E_- + E_0 = 1 \tag{1}$$

and it follows that $E_{\pm}$ may be expressed as $E_{\pm} = \alpha|\theta_{\perp}^{\mp}\rangle\langle\theta_{\perp}^{\mp}|$. Thus in the $|0\rangle$, $|1\rangle$ basis, we express the POVM relation (1) as the matrix equation

$$\begin{pmatrix} 2\alpha\sin^2(\theta/2) + E_{00} & E_{01} \\ E_{10} & 2\alpha\cos^2(\theta/2) + E_{11} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

where $E_{ij} \equiv \langle i|E_0|j\rangle$ for $i, j = 0, 1$. We immediately see the off-diagonal elements of E_0 must be zero and we are left with two equations:

$$E_{00} = 1 - 2\alpha\sin^2(\theta/2) \tag{2}$$

$$E_{11} = 1 - 2\alpha\cos^2(\theta/2). \tag{3}$$

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Setting each matrix element to zero and rearranging, we have

$$\frac{1}{2} = \alpha \sin^2(\theta/2) \tag{4}$$

$$\frac{1}{2} = \alpha \cos^2(\theta/2). \tag{5}$$

Adding the two equations together

$$1 = \alpha(\cos^2(\theta/2) + \sin^2(\theta/2)) = \alpha.$$

Substituting $\alpha = 1$ into (4) and (5) we see that for $\theta \in [0, \pi/2]$, the equations are only satisfied for $\theta = \pi/2$. Thus we have shown that $E_0 = 0$ only if $\alpha = 1$ and $\theta = \pi/2$.

Given that $E_0 > 0$ means that E_0 is positive operator (which includes the zero operator), it follows that the eigenvalues of E_0 must be non-negative. Thus we use E_0 in its diagonal form to give the following inequalities

$$1 - 2\alpha \sin^2(\theta/2) = 1 - 2\alpha(1 - \cos\theta) \le 0$$

$$\Rightarrow \alpha \le \frac{1}{1 + \cos\theta}$$

and

$$1 - 2\alpha \cos^2(\theta/2) = 1 - 2\alpha(1 + \cos\theta) \le 0$$

$$\Rightarrow \alpha \le \frac{1}{1 - \cos\theta}.$$

For $\theta \in [0, \pi/2]$

$$\frac{1}{1 + \cos\theta} \le \frac{1}{1 - \cos\theta}$$

and so

$$\alpha \le \frac{1}{1 + \cos\theta} \le \frac{1}{1 - \cos\theta}.$$

Thus for $E_0 > 0$ we must have $\alpha \le 1/(1 + \cos\theta)$.

(b) Let us first compute the probabilities $P_{\pm}$:

$$P_{\pm} = \langle \theta^{\pm} | E_0 | \theta^{\pm} \rangle$$

$$= \begin{pmatrix} \cos(\theta/2) & \pm\sin(\theta/2) \end{pmatrix} \begin{pmatrix} 1 - 2\alpha\sin^2(\theta/2) & 0 \\ 0 & 1 - 2\alpha\cos^2(\theta/2) \end{pmatrix} \begin{pmatrix} \cos(\theta/2) \\ \pm\sin(\theta/2) \end{pmatrix}$$

$$= 1 - 4\alpha[\sin^2(\theta/2)\cos^2(\theta/2)]$$

$$= 1 - \alpha\sin^2\theta.$$

Given our range of α and θ, the probability $P_{\pm}$ can only be zero for $\alpha = 1$, $\theta = \pi/2$ (easy to see from bounds of $\sin^2\theta$). But these are precisely the conditions for $E_0 = 0$, which we take as false from the outset of this problem. Thus we have shown for $E_0 \ne 0$, $P_{\pm} \ne 0$. Note that for $\theta < \pi/2$ we have a non-zero probability for measuring ambiguous outcome "0".

(c) From part (b),
$$P_{\pm} = 1 - \alpha\sin^2\theta.$$

Since E_0 is a positive operator we may substitute our relation for α in part (a)

$$\alpha \le \frac{1}{1 + \cos\theta}$$

$$1 - \alpha \sin^2 \theta \geq 1 - \frac{\sin^2 \theta}{1 + \cos \theta}$$

$$P_\pm \geq \cos \theta$$

Thus the minimal probability for an ambiguous result occurs at $\cos \theta$.

2. Let us study relaxation terms in the two-level system as in the text, except that we generically denote the damping rates of the coherences by γ, not specifically $\Gamma/2$. In this example, also ignore the Liouville-von Neumann part of the time evolution, which has no effect on the present results anyway. Thus we have

$$\dot{\rho}_{11} = -\Gamma \rho_{11}, \ \dot{\rho}_{00} = \Gamma \rho_{11}, \ \dot{\rho}_{10} = -\gamma \rho_{10}, \ \dot{\rho}_{01} = -\gamma \rho_{01}.$$

(a) By studying the time evolution of the density matrix ρ_{ij} starting from a pure state, show that unless $\gamma \geq \Gamma/2$, a density matrix can always be found that does not stay positive under this time evolution.

(b) In contrast, when $\gamma \geq \Gamma/2$, a positive density matrix always stays positive. Show this by giving Linblad operators from which you can derive the relaxation terms for this case.

(a) I will take the statement "unless A, there exists a B" as equilvalent to "if $\bar{A}$ then B", where $A \equiv \gamma \geq \Gamma/2$ and B denotes the existence of a non-positive density matrix.

Denoting the matrix elements $\langle i | \rho | j \rangle = \rho_{ij}$ for $i, j = 0, 1$ we may form the matrix of our density operator in the basis of our two-level system:

$$\rho(t) = \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix}.$$

We seek to find a condition of positivity for this matrix. This can be accomplished by the following arguments. First note that the eigenvalues of a pure state are 0 and 1. Then, by being hermitian, the determinant of the density matrix is given by the product of eigenvalues. Thus

$$\det[\rho(t)] = \rho_{00}(t)\rho_{11}(t) - \rho_{01}(t)\rho_{10}(t) = \prod_{i=0,1} \lambda_i = 0$$

$$\Rightarrow \rho_{00}(t)\rho_{11}(t) = \rho_{01}(t)\rho_{10}(t). \tag{6}$$

If our system starts in the pure state at time t, then $\det[\rho(t)] = 0$. If at a subsequent time t', $\det[\rho(t')] < 0$, then it follows that

$$\left(\frac{d}{dt} \det[\rho(t)] \right) \bigg|_\tau < 0$$

for some time $t \leq \tau \leq t'$. Since the determinant was at negative at t', this implies it was not a positive matrix. As such, the derivative of the determinant serves as a possible condition of positivity.

Proceeding with the determinant

$$\begin{aligned} \frac{d}{dt} \det[\rho(t)] &= \frac{d}{dt} [\rho_{00}(t)\rho_{11}(t) - \rho_{01}(t)\rho_{10}(t)] \\ &= \dot{\rho}_{00}(t)\rho_{11}(t) + \rho_{00}(t)\dot{\rho}_{11}(t) - \dot{\rho}_{01}(t)\rho_{10}(t) - \rho_{01}(t)\dot{\rho}_{10}(t) \\ &= \Gamma \rho_{11}(t)^2 - \Gamma \rho_{00}(t)\rho_{11}(t) + 2\gamma \rho_{01}(t)\rho_{10}(t) \\ &= \Gamma \rho_{11}(t)^2 - \Gamma \rho_{00}(t)\rho_{11}(t) + 2\gamma \rho_{00}(t)\rho_{11}(t) \\ &= \rho_{11}(t) \left(\Gamma \rho_{11}(t) + (2\gamma - \Gamma)\rho_{00}(t) \right) \end{aligned}$$

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If $\gamma < \Gamma/2$ we see that there clearly exists a $\rho_{00}(t)$ such that the derivative becomes negative, and so our density operator is non-positive.

(b) Time evolution following the Lindblad form goes as

$$\dot{\rho} = \mathcal{L}\rho = \sum_k [2L_k \rho L_k^\dagger - L_k^\dagger L_k \rho - \rho L_k^\dagger L_k].$$

To attempt to recover the relaxation terms as given in the problem, let us first take the Lindblad operators

$$L_1 = \sqrt{\frac{\Gamma}{2}} \, |0\rangle \langle 1|, \qquad L_1^\dagger = \sqrt{\frac{\Gamma}{2}} \, |1\rangle \langle 0|$$

and

$$L_2 = \beta \, |1\rangle \langle 1|, \qquad L_2^\dagger = \beta^* \, |1\rangle \langle 1|.$$

Then evolving over time,

$$\dot{\rho} = \mathcal{L}\rho$$
$$= \frac{\Gamma}{2}(2 \, |0\rangle \langle 1|\rho|1\rangle \langle 0| - |1\rangle \langle 1| \, \rho - \rho \, |1\rangle \langle 1|)$$
$$+ |\beta|^2 (2 \, |1\rangle \langle 1|\rho|1\rangle \langle 1| - |1\rangle \langle 1| \, \rho - \rho \, |1\rangle \langle 1|).$$

Now take the matrix elements

$$\dot{\rho}_{00} = \Gamma \, \langle 1|\rho|1\rangle = \Gamma \rho_{11}$$

$$\dot{\rho}_{01} = -\left(\frac{\Gamma}{2} + |\beta|^2\right) \langle 0|\rho|1\rangle = -\left(\frac{\Gamma}{2} + |\beta|^2\right) \rho_{01}$$

$$\dot{\rho}_{10} = -\left(\frac{\Gamma}{2} + |\beta|^2\right) \langle 1|\rho|0\rangle = -\left(\frac{\Gamma}{2} + |\beta|^2\right) \rho_{10}$$

$$\dot{\rho}_{11} = -\Gamma \, \langle 1|\rho|1\rangle = -\Gamma \rho_{11}.$$

If we choose β such that

$$\beta = \sqrt{\gamma - \frac{\Gamma}{2}} \qquad \text{where} \qquad \gamma \geq \frac{\Gamma}{2}$$

then $\beta \in \mathbb{R}$ and

$$|\beta|^2 = \left(\gamma - \frac{\Gamma}{2}\right).$$

This yields the proper relaxation terms

$$\dot{\rho}_{11} = -\Gamma \rho_{11}, \quad \dot{\rho}_{00} = \Gamma \rho_{11}, \quad \dot{\rho}_{10} = -\gamma \rho_{10}, \quad \dot{\rho}_{01} = -\gamma \rho_{01}$$

Since they follow the Lindblad form, we are guaranteed that the map $\mathcal{L}$ acting upon ρ is positive and trace preserving. To recap, for $\gamma \geq \frac{\Gamma}{2}$ we may always form Lindblad operators that give the appropriate relaxation terms, and thus our positive density matrix remains positive.

3. To avoid inessential complications, think of a one-component Fermi gas with the field operator $\psi(\mathbf{r})$.

   (a) Show that $\psi(\mathbf{r})\psi(\mathbf{r}) = 0$.
   (b) Take the positions $\mathbf{r}_i, i = 1, \cdots, N$, all distinct: $i \neq j \implies \mathbf{r}_i \neq \mathbf{r}_j$. Argue that the state $|\psi\rangle = \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\cdots\psi^\dagger(\mathbf{r}_N)|0\rangle$ plausibly is a state with one particle at each position $\mathbf{r}_1, \cdots, \mathbf{r}_N$.

(c) Why does the condition $i \neq j \implies \mathbf{r}_i \neq \mathbf{r}_j$ matter?

(a) Starting with the construction of the field operator

$$\psi(\mathbf{r}) = \sum_k u_k(\mathbf{r})a_k, \qquad \text{where} \qquad \{a_k, a_{k'}^\dagger\} = \delta_{kk'}$$

it follows that

$$\psi(\mathbf{r})\psi(\mathbf{r}) = \sum_{k,k'} u_k(\mathbf{r})u_k'(\mathbf{r})a_k a_k'$$

$$= -\sum_{k,k'} u_k(\mathbf{r})u_k'(\mathbf{r})a_k' a_k$$

$$= -\psi(\mathbf{r})\psi(\mathbf{r})$$

where we have used the anticommutation for a_k, a_k'. From the above, we must conclude

$$\psi(\mathbf{r})\psi(\mathbf{r}) = 0.$$

(b) First, let us construct a general identity regarding anticommutators. From the two relations

$$[A, BC] = \{A, B\}C - B\{A, C\}$$

and

$$\{A, BC\} = \{A, B\}C - B[A, C],$$

we may construct the anticommutation of a product of operators:

$$\{a_1, a_2 a_3...a_n\} = \{a_1, a_2\}a_3...a_n - a_2[a_1, a_3...a_n]$$
$$= \{a_1, a_2\}a_3...a_n - a_2\left(\{a_1, a_3\}a_4...a_n - a_3\{a_1, a_4...a_n\}\right)$$
$$= \{a_1, a_2\}a_3...a_n - a_2\{a_1, a_3\}a_4...a_n + a_2 a_3\{a_1, a_4\}a_5...a_n - a_2 a_3 a_4\{a_1, a_5\}a_6...a_n + ...$$

Note that we pick up a minus sign when we have an odd number of operators to the left of the anticommutator.

With this relation in hand, we proceed to apply the number operator to our state and take an anticommutator

$$\hat{n}(\mathbf{R})\,|\psi\rangle = \psi^\dagger(\mathbf{R})\psi(\mathbf{R})\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)...\psi^\dagger(\mathbf{r}_N)\,|0\rangle$$

$$= \psi^\dagger(\mathbf{R})\left(\{\psi(\mathbf{R}), \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)...\psi^\dagger(\mathbf{r}_N)\} - \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)...\psi^\dagger(\mathbf{r}_N)\psi(\mathbf{R})\right)|0\rangle$$

$$= \psi^\dagger(\mathbf{R})\left(\{\psi(\mathbf{R}), \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)...\psi^\dagger(\mathbf{r}_N)\}\right)|0\rangle$$

$$= \psi^\dagger(\mathbf{R})\left(\{\psi(\mathbf{R}), \psi^\dagger(\mathbf{r}_1)\}\psi^\dagger(\mathbf{r}_2)...\psi^\dagger(\mathbf{r}_n) - \psi^\dagger(\mathbf{r}_1)\{\psi(\mathbf{R}), \psi^\dagger(\mathbf{r}_2)\}\psi^\dagger(\mathbf{r}_3)...\psi^\dagger(\mathbf{r}_n)\right.$$

$$\left. + \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\{\psi(\mathbf{R}), \psi^\dagger(\mathbf{r}_3)\}\psi^\dagger(\mathbf{r}_4)...\psi^\dagger(\mathbf{r}_n) - ...\right)|0\rangle$$

$$= \psi^\dagger(\mathbf{R})\left(\delta(\mathbf{R} - \mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)..\psi^\dagger(\mathbf{r}_n) - \delta(\mathbf{R} - \mathbf{r}_2)\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_3)..\psi^\dagger(\mathbf{r}_n)\right.$$

$$\left. + \delta(\mathbf{R} - \mathbf{r}_3)\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\psi^\dagger(\mathbf{r}_4)..\psi^\dagger(\mathbf{r}_n) - ...\right)|0\rangle$$

$$= \Big(\delta(\mathbf{R} - \mathbf{r}_1)\psi^\dagger(\mathbf{r}_1)...\psi^\dagger(\mathbf{r}_n) - \delta(\mathbf{R} - \mathbf{r}_2)\psi^\dagger(\mathbf{r}_2)\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_3)...\psi^\dagger(\mathbf{r}_n)$$

$$+ \delta(\mathbf{R} - \mathbf{r}_3)\psi^\dagger(\mathbf{r}_3)\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\psi^\dagger(\mathbf{r}_4)...\psi^\dagger(\mathbf{r}_n) - ... \Big) |0\rangle$$

$$= \sum_i \delta(\mathbf{R} - \mathbf{r}_i)\psi^\dagger(\mathbf{r}_1)...\psi^\dagger(\mathbf{r}_n) |0\rangle$$

$$\hat{n}(\mathbf{R}) |\psi\rangle = \sum_i \delta(\mathbf{R} - \mathbf{r}_i) |\psi\rangle$$

where in the third to last line we used the anticommutation relation $\{\psi^\dagger(\mathbf{r}_i), \psi^\dagger(\mathbf{r}_j)\} = 0$. This worked nicely because the minus signs are canceled exactly by the odd number of anticommutation operations.

We see that $|\psi\rangle$ is an eigenstate of the number operator with a non-zero eigenvalue only for $\mathbf{R} = \mathbf{r}_i$. This suggests the state $|\psi\rangle$ consists of a collection of quanta localized in space at each $\mathbf{r}_i$. We tend to call these particles.

(c) By an analogous argument as that of part (a), we may easily show $\psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}) = 0$. This suggests that we cannot place two quanta at the same localized position. This result is specific to fermions (well, excluding a particular 1D Bose gas) and is in accordance with the Pauli exclusion principle. That is, since we take the state of a fermion system to be antisymmetric with respect to particle exchange, it follows that two fermions may not occupy the same position.

4. In a simplified but justifiable (never mind the details) model for conversion of two species of fermionic atoms ($c_{\mathbf{k}\uparrow}, c_{\mathbf{k}\downarrow}$) to bosonic molecules ($b$) one may write the Hamiltonian

$$\frac{H}{\hbar} = \sum_{\mathbf{k},\sigma} \omega_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \delta b^\dagger b + \xi \sum_{\mathbf{k}} (b^\dagger c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + c^\dagger_{-\mathbf{k}\downarrow} c^\dagger_{\mathbf{k}\uparrow} b)$$

(a) Verify the Heisenberg equations of motion

$$\dot{b} = -i\delta b - i\xi \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}, \quad \dot{c}_{\mathbf{k}\uparrow} = -i\omega_k c_{\mathbf{k}\uparrow} + i\xi b c^\dagger_{-\mathbf{k}\downarrow}, \quad \dot{c}_{-\mathbf{k}\downarrow} = -i\omega_k c_{-\mathbf{k}\downarrow} - i\xi b c^\dagger_{\mathbf{k}\uparrow}.$$

(b) Find the Heisenberg equations of motion for the operators $c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow}$, $c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}\downarrow}$, and $c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}$.

(c) You cannot make a mean field approximation for fermion operators, but at low temperatures when a BEC of the molecules is possible you may approximate the operator b with a corresponding c-number β. You then find a closed set of equations for the amplitude β, the expectation values of the occupation numbers $P_\uparrow(\mathbf{k}) = \langle c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}\uparrow} \rangle$, and for the pairing amplitudes $C(\mathbf{k}) = \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$. Do it!

You have here the essence of what is called two-channel theory of BEC-BCS crossover.

(a) Starting with the boson operator

$$\dot{b} = -i[b, H]$$

$$= -i \left(\delta[b, b^\dagger b] + \xi \sum_{\mathbf{k}} [b, b^\dagger](c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}) \right)$$

$$\boxed{\dot{b} = -i\delta b - i\xi \sum_{\mathbf{k}} c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow}}.$$

Spin up fermion operator:

$$\dot{c}_{\mathbf{k}\uparrow} = -i\left[\sum_{\mathbf{k'}}\omega'_k([c_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k'}\uparrow}c_{\mathbf{k'}\uparrow}] + [c_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k'}\downarrow}c_{\mathbf{k'}\downarrow}]) + \xi\sum_{\mathbf{k'}}\left(b^\dagger[c_{\mathbf{k}\uparrow},c_{\mathbf{k'}\uparrow}c_{-\mathbf{k'}\downarrow}] + [c_{\mathbf{k}\uparrow},c^\dagger_{-\mathbf{k'}\downarrow}c^\dagger_{\mathbf{k'}\uparrow}]b)\right]$$

$$= -i\left[\sum_{\mathbf{k'}}\omega'_k\left(\{c_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k'}\uparrow}\}c_{\mathbf{k'}\uparrow} - c^\dagger_{\mathbf{k'}\uparrow}\{c_{\mathbf{k}\uparrow},c_{\mathbf{k'}\uparrow}\} + \{c_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k'}\downarrow}\}c_{\mathbf{k'}\downarrow} - c^\dagger_{\mathbf{k'}\downarrow}\{c_{\mathbf{k}\uparrow},c_{\mathbf{k'}\downarrow}\}\right)\right.$$

$$\left. + \xi\sum_{\mathbf{k'}}\left(\{c_{\mathbf{k}\uparrow},c^\dagger_{-\mathbf{k'}\downarrow}\}c^\dagger_{\mathbf{k'}\uparrow}b - c^\dagger_{-\mathbf{k}\downarrow}\{c_{\mathbf{k}\uparrow},c^\dagger_{\mathbf{k'}\uparrow}\}b\right)\right]$$

$$= -i\sum_{\mathbf{k'}}\omega'_k c_{\mathbf{k'}\uparrow}\delta_{\mathbf{k}\mathbf{k'}} + i\xi\sum_{\mathbf{k'}}c^\dagger_{-\mathbf{k'}\downarrow}b\delta_{\mathbf{k}\mathbf{k'}}$$

$$\boxed{\dot{c}_{\mathbf{k}\uparrow} = -i\omega_k c_{\mathbf{k}\uparrow} + i\xi b c^\dagger_{-\mathbf{k}\downarrow}}.$$

And similarly for the spin down $(-\mathbf{k})$:

$$\dot{c}_{-\mathbf{k}\downarrow} = -i\left[\sum_{\mathbf{k'}}\omega'_k([c_{-\mathbf{k}\downarrow},c^\dagger_{\mathbf{k'}\uparrow}c_{\mathbf{k'}\uparrow}] + [c_{-\mathbf{k}\downarrow},c^\dagger_{\mathbf{k'}\downarrow}c_{\mathbf{k'}\downarrow}]) + \xi\sum_{\mathbf{k'}}\left(b^\dagger[c_{-\mathbf{k}\downarrow},c_{\mathbf{k'}\uparrow}c_{-\mathbf{k'}\downarrow}] + [c_{-\mathbf{k}\downarrow},c^\dagger_{-\mathbf{k'}\downarrow}c^\dagger_{\mathbf{k'}\uparrow}]b)\right]$$

$$= -i\left[\sum_{\mathbf{k'}}\omega'_k\left(\{c_{-\mathbf{k}\downarrow},c^\dagger_{\mathbf{k'}\downarrow}\}c_{\mathbf{k'}\downarrow} - c^\dagger_{\mathbf{k'}\downarrow}\{c_{-\mathbf{k}\downarrow},c_{\mathbf{k'}\downarrow}\}\right) + \xi\sum_{\mathbf{k'}}\left(\{c_{-\mathbf{k}\downarrow},c^\dagger_{-\mathbf{k'}\downarrow}\}c^\dagger_{\mathbf{k'}\uparrow}b - c^\dagger_{-\mathbf{k}\downarrow}\{c_{-\mathbf{k}\downarrow},c^\dagger_{\mathbf{k'}\uparrow}\}b\right)\right]$$

$$= -i\sum_{\mathbf{k'}}\omega'_k c_{\mathbf{k'}\downarrow}\delta_{-\mathbf{k}\mathbf{k'}} - i\xi\sum_{\mathbf{k'}}c^\dagger_{\mathbf{k'}\uparrow}b\delta_{\mathbf{k}\mathbf{k'}}$$

$$\boxed{\dot{c}_{-\mathbf{k}\downarrow} = -i\omega_k c_{-\mathbf{k}\downarrow} - i\xi b c^\dagger_{\mathbf{k}\uparrow}}$$

(b) Lets start with $c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}$:

$$\frac{d}{dt}(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}) = \dot{c}^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\uparrow}\dot{c}_{\mathbf{k}\uparrow}$$

$$= (i\omega_k c^\dagger_{\mathbf{k}\uparrow} - i\xi b^\dagger c_{-\mathbf{k}\downarrow})c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\uparrow}(-i\omega_k c_{\mathbf{k}\uparrow} + i\xi b c^\dagger_{-\mathbf{k}\downarrow})$$

$$= -i\xi(b^\dagger c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} - b c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow})$$

$$\boxed{\frac{d}{dt}(c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow}) = i\xi(b^\dagger c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} - b c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow})}.$$

Now for $c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow}$:

$$\frac{d}{dt}(c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow}) = \dot{c}^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow} + c^\dagger_{-\mathbf{k}\downarrow}\dot{c}_{-\mathbf{k}\downarrow}$$

$$= (i\omega_k c^\dagger_{-\mathbf{k}\downarrow} + i\xi b^\dagger c_{\mathbf{k}\uparrow})c_{-\mathbf{k}\downarrow} + c^\dagger_{-\mathbf{k}\downarrow}(-i\omega_k c_{-\mathbf{k}\downarrow} - i\xi b c^\dagger_{\mathbf{k}\uparrow})$$

$$\boxed{\frac{d}{dt}(c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow}) = i\xi(b^\dagger c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} - b c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow})}$$

Lastly for $c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}$:

$$\frac{d}{dt}(c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}) = \dot{c}_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} + c_{\mathbf{k}\uparrow}\dot{c}_{-\mathbf{k}\downarrow}$$

$$= (-i\omega_k c_{\mathbf{k}\uparrow} + i\xi b c^\dagger_{-\mathbf{k}\downarrow})c_{-\mathbf{k}\downarrow} + c_{\mathbf{k}\uparrow}(-i\omega_k c_{-\mathbf{k}\downarrow} - i\xi b c^\dagger_{\mathbf{k}\uparrow})$$

$$= -2i\omega_k c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} + i\xi b(c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow} - c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k}\uparrow})$$

$$\boxed{\frac{d}{dt}(c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}) = -2i\omega_k c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} + i\xi b(c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow} - c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k}\uparrow})}$$

(c) Relevant equation for the time derivative of expectation values:

$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle [A, H] \rangle = \langle \dot{A} \rangle,$$

assuming no explicit time dependence. We take the operator

$$b \to \beta \in \mathbb{C}$$

then it follows that

$$
\begin{aligned}
\frac{d}{dt}P_\uparrow(\mathbf{k}) &= \frac{d}{dt}P_\downarrow(\mathbf{k}) \\
&= \frac{d}{dt}\langle c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} \rangle \\
&= i\xi \langle b^\dagger c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} - bc^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow} \rangle \\
&= i\xi(\beta^* \langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} \rangle - \beta \langle c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow} \rangle) \\
&= i\xi(\beta^* C(\mathbf{k}) - \beta C^*(\mathbf{k}))
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}C(\mathbf{k}) &= \frac{d}{dt}\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} \rangle \\
&= \langle -2i\omega_k c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} + i\xi b(c^\dagger_{-\mathbf{k}\downarrow}c_{-\mathbf{k}\downarrow} - c_{\mathbf{k}\uparrow}c^\dagger_{\mathbf{k}\uparrow}) \rangle \\
&= -2i\omega_k C(\mathbf{k}) + i\xi\beta(P_\downarrow(\mathbf{k}) + P_\uparrow(\mathbf{k}) - 1)
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}\langle b \rangle &= -i\delta\beta - i\xi \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow} \rangle \\
&= -i\delta\beta - i\xi \sum_{\mathbf{k}} C(\mathbf{k}) \\
&= 0.
\end{aligned}
$$

Thus we end up with the following three equations

$$\beta = -\frac{\xi}{\delta}\sum_{\mathbf{k}}C(\mathbf{k}) \tag{7}$$

$$\frac{d}{dt}P_{\uparrow,\downarrow}(\mathbf{k}) = i\xi[\beta^* C(\mathbf{k}) - \beta C^*(\mathbf{k})] \tag{8}$$

$$\frac{d}{dt}C(\mathbf{k}) = -2i\omega C(\mathbf{k}) + i\xi\beta[P_\uparrow(\mathbf{k}) + P_\downarrow(\mathbf{k}) - 1]. \tag{9}$$

To see that these are indeed closed, one approach may be to take the second derivative of (9), substitute in derivates from (8) and then substitute equation (7) for β. This gives a closed form second order differential equation for $C(\mathbf{k})$. Once solved, β is then defined, and subsequently $P_{\uparrow,\downarrow}(\mathbf{k})$ may be solved as a first order equation. The only trouble I see here is that our $C(\mathbf{k})$ differential equation will be defined in terms of a summation of different $\mathbf{k}$ modes.

5. Let us study a trapped Bose-Einstein condensate of N atoms with contact interactions (scattering length a) in an isotropic harmonic oscillator potential ($U = \frac{1}{2}m\omega^2\mathbf{r}^2$) semiclassically using a *variational* ansatz for the macroscopic wave function $\psi(\mathbf{r})$, or the form

$$\psi(\mathbf{r}) \propto \exp\left[-\frac{\mathbf{r}^2}{4L^2}\right].$$

The variational parameter L is the root-mean square width of the condensate in the x (and y and z) direction.

(a) Show that in the harmonic oscillator units (with $\hbar = m = \omega = 1$) the energy per particle of the condensate is

$$\frac{E}{N} = \frac{3L + 12L^5 + 2aN/\sqrt{\pi}}{8L^3}$$

(b) This line of reasoning suggests that if the scattering length is negative, the condensate collapses if the atom number is large enough, namely if

$$N \geq \frac{2^{3/2}\pi^{1/2}}{5^{5/4}|a|} \simeq \frac{0.67}{|a|}.$$

Here, too, a is in the harmonic oscillator units; with all of the dimensional parameters restored, we would have $\left|a/\sqrt{\hbar/m\omega}\right|$ in the denominator. Produce the full argument.

Even if the result is not necessarily numerically very accurate, it is found empirically that a trapped condensate with a negative scattering length appears to be stable up to some critical atom number, and promptly disappears at higher atom numbers.

(c) What is the qualitative physics: What stabilizes the condensate against collapse for small atom numbers, and why does the atom number make a difference?

(a) We may calculate the energy of the BEC via the Kamiltonian,

$$K = H - \mu N$$

where, instead of proceeding with second quantization, we semi-classically compute the observables using the macroscopic wavefunction

$$\psi(\mathbf{r}) = C \exp\left[-\frac{\mathbf{r}^2}{4L^2}\right].$$

Accordingly, the Kamiltonian consists of the kinetic energy, chemical potential, and atom-atom interaction energy, given by

$$H - \mu N = \int dV \; \psi^\dagger \left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 - \mu\right)\psi + \frac{2\pi a\hbar^2}{m}\int dV \; \psi^\dagger\psi^\dagger\psi\psi.$$

In our natural harmonic oscillator units, this is then

$$K = 4\pi C^2 \int_0^\infty dr \; r^2 \left(\exp\left[-\frac{r^2}{2L^2}\right]\left(\frac{r^2 - 6L^2}{4L^4} + \frac{1}{2}r^2 - \mu\right)\right) + 4\pi(2\pi a)C^4 \int dr \; r^2 \exp\left[-\frac{r^2}{L^2}\right]$$

$$= 2\sqrt{2}(\pi^{3/2})C^2 \left[L^3\left(\frac{3}{2}L^2 - \mu + \frac{\sqrt{2}}{2}\pi a C^2\right) + \frac{3}{8}L\right].$$

From here, we explicitly substitute our normalization,

$$\int dV \; \psi^\dagger\psi = N \quad \Rightarrow \quad C^2 = \frac{N}{2\sqrt{2}\pi^{3/2}L^3},$$

into the Kamiltonian

$$K = N \left[\frac{3}{2}L^2 - \mu + \frac{aN}{4L^3\sqrt{\pi}} \right] + \frac{3N}{8L^2}.$$

Then, the energy is easily found as

$$E = K + \mu N$$

in which the energy per particle is

$$\frac{E}{N} = \left[\frac{3}{2}L^2 + \frac{aN}{4\sqrt{\pi}L^3} \right] + \frac{3}{8L^2},$$

which simplifies to

$$\boxed{\frac{E}{N} = \frac{3L + 12L^5 + 2aN/\sqrt{\pi}}{8L^3}}.$$

(b) As we take $L \to \infty$, the energy per particle becomes very large. However, the behavior as $L \to 0$ depends on the strength and sign of the aN term. For scattering length $a \geq 0$ (repulsive interaction), the energy assumes a stable equilibrium at a minimum, as depicted below:

aN ≥ 0
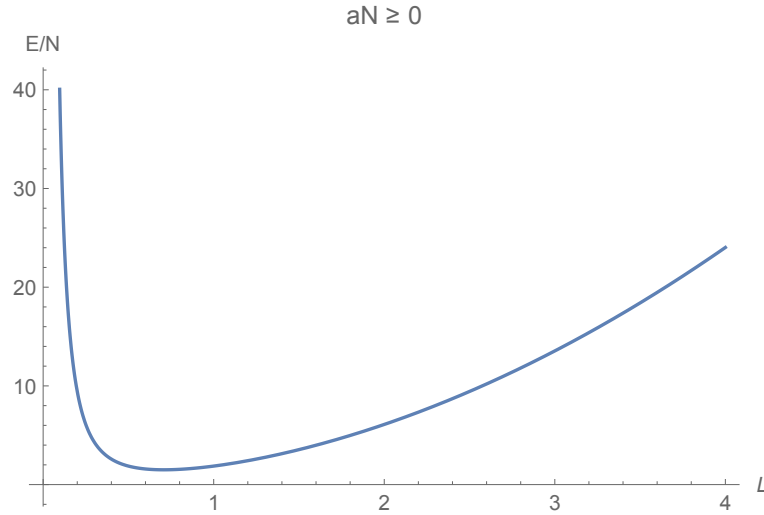
However for a negative scattering length $a < 0$ (attractive interaction), the local minimum disappears at a critical $aN \leq \lambda_c$. Here is an illustration as aN decreases:

$\lambda_c < aN < 0$

$aN = \lambda_c$

$aN < \lambda_c$
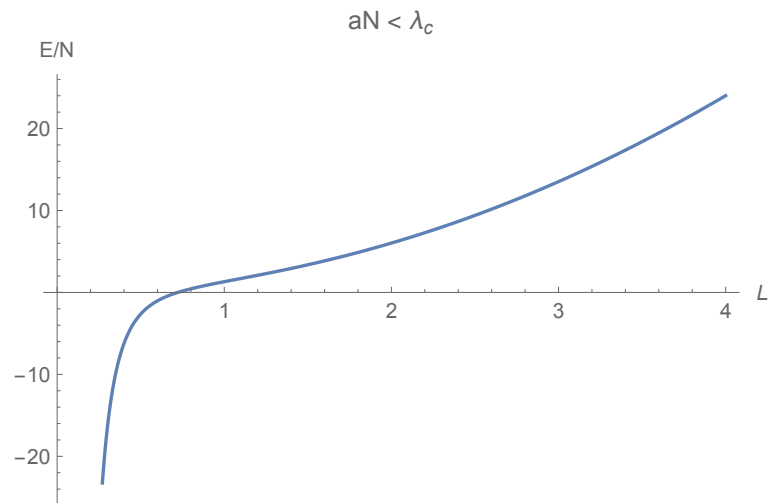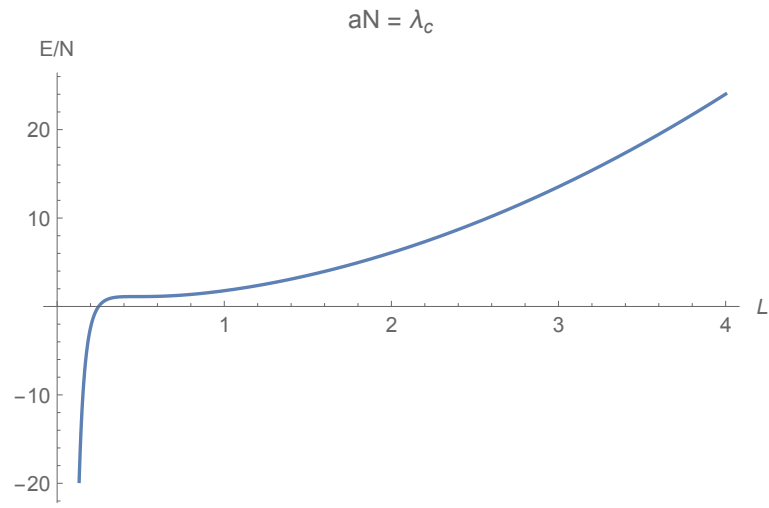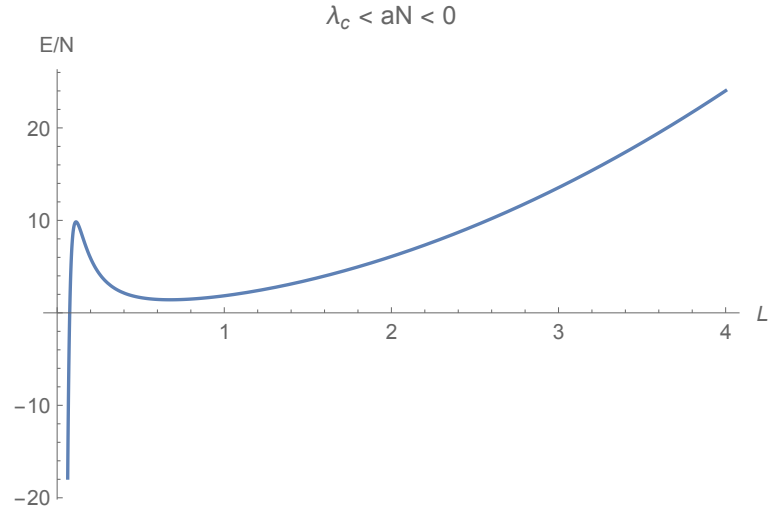
The critical point corresponds to a minimum with a saddle point inflection. For a fixed (negative) scattering

length, the critical density can be found by taking first and second derivatives of the energy to zero:

$$\frac{d}{dL}\left(\frac{E}{N}\right)\bigg|_{aN_c} = \frac{3}{4}\left(\frac{L^5 - L - \frac{aN}{\sqrt{\pi}}}{L^4}\right)\bigg|_{aN_c} = 0$$

$$\frac{d^2}{dL^2}\left(\frac{E}{N}\right)\bigg|_{aN_c} = \left(3 + \frac{9}{4L^4} + \frac{3aN}{\sqrt{\pi}L^5}\right)\bigg|_{aN_c} = 0.$$

Solving these two equations simultaneously for aN_c, we find

$$aN_c = -\frac{2^{3/2}\pi^{1/2}}{5^{5/4}}.$$

As evident from the graphs, for $N \geq N_c$, the energy per particle becomes unbounded from below and the BEC becomes unstable (collapses). Thus our condition for the onset of instability is then

$$|a|N \geq \frac{2^{3/2}\pi^{1/2}}{5^{5/4}} \simeq 0.67$$

(c) Given our confining harmonic potential, the kinetic energy of the BEC ground state counteracts the attractive scattering potential and effectively stabilizes the condensate. This is true only for small enough attractive interactions. As the the attractive interaction energy increases, i.e. by adding more atoms or increasing $|a|$, the attractive interaction will eventually overcome the kinetic energy and make the condensate unstable.