Lecture 32

Today show you an example of how some of the
ideas we've been talking about get applied to
real problems.

Talk about the effect of interactions in a Bose
condensate

Warning: this is somewhat advanced. I think you'll be
able to follow the gist & find it interesting,
but I won't give HW on it or have anything like
this on the final.

So, our question is:
   What is ground state for N interacting bosons
      in a potential $U(r)$? Interaction potential $u(r)$

Hamiltonian is

$$H = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + U(r_i) \right] + \frac{1}{2} \sum_{j \neq i} u(|r_i - r_j|)$$

   Wave function $\Psi(r_1, r_2, \ldots r_N)$

Try variational approach.

   With no interactions, $\Psi = \phi_0(r_1) \phi_0(r_2) \ldots \phi_0(r_N)$

                        $\phi_0 =$ single particle ground state

   Try $\Psi = \phi(r_1) \phi(r_2) \ldots \phi(r_N)$

      Pick ϕ to satisfy variational condition
         - note this is a function, not a single parameter

First evaluate $\langle H \rangle = \langle \Psi | H | \Psi \rangle$

$$= \int dr_1 \, dr_2 \dots dr_N \; \phi_1^* \phi_2^* \dots \phi_N^*$$
$$\times \left\{ \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(r_i) \right] + \frac{1}{2} \sum_{i \neq j} U(|r_i - r_j|) \right\}$$
$$\times \phi_1 \phi_2 \dots \phi_N$$

$\phi_1 \equiv \phi(r_1)$ etc

$$= \sum_i \int dr_i \; \phi_i^* \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(r_i) \right] \phi_i$$

$$+ \frac{1}{2} \sum_{i,j} \int dr_i \, dr_j \; \phi_i^* \phi_j^* \, U(|r_i - r_j|) \phi_i \phi_j$$

But we can relabel integration variables as we like

$$\langle H \rangle = N \int dr \; \phi^*(r) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \phi(r)$$

$$+ \frac{N(N-1)}{2} \int dr_1 \, dr_2 \; \phi^*(r_1) \phi^*(r_2) \, U(|r_1 - r_2|) \phi(r_1) \phi(r_2)$$

$\uparrow$
\# of pairs

That's a bit simpler

We want to minimize this with respect to ϕ, a function

Use variational calculus
    Will see in phys 321 if you haven't already

I'll try to explain it.

Idea: say we changed $\phi(r)$ to $\phi + \delta\phi(r)$
                    arbitrary but small $\delta\phi$

        Want $\langle H \rangle$ to be unchanged, to
                  first order in $\delta\phi$

First consider non interacting case $u=0$

$$H \rightarrow H_0$$

Then $\delta \langle H_0 \rangle = N \int d^3r \, (\phi + \delta\phi)^* \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] (\phi + \delta\phi)$

$$= N \int d^3r \left\{ \begin{array}{ll} \phi^* [\quad] \phi & \text{(indep of } \delta\phi) \\ + \delta\phi^* [\quad] \phi & \\ + \phi^* [\quad] \delta\phi & \end{array} \right\} \text{keep these}$$
$$+ \delta\phi^* [\quad] \delta\phi \Big\} \quad \text{(2nd order in } \delta\phi)$$

Third line has $\phi^* \nabla^2 \delta\phi$ term

integrate by parts twice to make this $\delta\phi \nabla^2 \phi^*$

(demand $\delta\phi \rightarrow 0$ for $r \rightarrow \infty$ anyway)

So

$$\delta \langle H_0 \rangle = N \int d^3r \left\{ \delta\phi^* \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \phi + \delta\phi \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \phi^* \right\}$$

Want $\delta \langle H_0 \rangle = 0$ for any $\delta\phi$ or $\delta\phi^*$

only possible if coefficients vanish

So need $\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \phi = 0$ (+ complex conj.)

Like regular Sch Eqn, but what about RHS?

Note, this is solved only by $\phi = 0$

which sure does minimize $\langle H_0 \rangle$

But we want to maintain normalization of ϕ.

We want to minimize $\langle H_0 \rangle$ subject to constraint

that $\int |\phi|^2 d^3r = 1$

In general, to minimize a function subject to a constraint, use Lagrange multipliers

Reminder: Minimize $f(x)$ subject to $g(x) = 0$
by minimizing
$$[f(x) - \mu g(x)]$$
to get $x_{min}(\mu)$

Then pick μ so that $g(x_{min}) = 0$ as desired

Here convenient to minimize

$$\langle H \rangle - \mu N (\langle \psi | \psi \rangle - 1)$$

$$= \langle H - \mu N \rangle - \underbrace{\mu N}_{\text{doesn't depend on } \psi, \text{ ignore}}$$

Follow same steps as before, get

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V - \mu \right) \phi = 0$$

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \phi = \mu \phi$$

So μ = energy of single particle state
Needs to be right, else ϕ not normalizable, makes sense

So that works out as expected for non interacting atoms. Put in interactions.

Get

$$\delta \langle u \rangle = \frac{N(N-1)}{2} \int\int [\phi_1^* + \delta\phi_1^*][\phi_2^* + \delta\phi_2^*] u(|r_1 - r_2|)$$
$$\times [\phi_1 + \delta\phi_1][\phi_2 + \delta\phi_2] \, d^3r_1 \, d^3r_2$$

Again, $\phi_1 = \phi(r_1)$ etc

Keep only linear terms

$$\delta\langle u \rangle \to \frac{N(N-1)}{2} \int\int d^3r_1 \, d^3r_2 \, u(|r_1-r_2|) \times$$
$$[\; \delta\phi_1^* \;\; \phi_2^* \;\; \phi_1 \;\; \phi_2$$
$$+ \phi_1^* \;\; \delta\phi_2 \;\; \phi_1 \;\; \phi_2$$
$$+ \phi_1^* \;\; \phi_2^* \;\; \delta\phi_1 \;\; \phi_2$$
$$+ \phi_1^* \;\; \phi_2^* \;\; \phi_1 \;\; \delta\phi_2 \;]$$
$$\Big\}\to \text{relable } 1 \leftrightarrow 2$$

becomes

$$N(N-1) \int\int d^3r_1 \, d^3r_2 \, u(|r_1-r_2|)[\delta\phi_1^* \phi_1 + \delta\phi_1 \phi_1^*]|\phi_2|^2$$

Or total

$$\delta\langle H \rangle = N \int d^3r_1 \left\{ \delta\phi_1^* \left[-\frac{\hbar^2}{2m}\nabla_1^2 + V(r_1) - \mu + (N-1)\int d^3r_2 \, u(|r_1-r_2|)|\phi_2|^2 \right] \right.$$
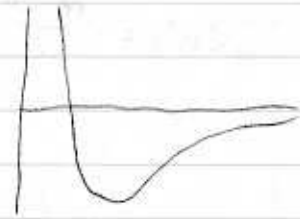$$\left. \times \phi_1 \right\} + \text{complex conjugate}$$

So now we need

$$\left\{ -\frac{\hbar^2}{2m}\nabla^2 + V(r) + (N-1)\left[\int d^3r' \, u(|r-r'|) |\phi(r')|^2\right] \right\}\phi = \mu\phi$$

So this is an equation we could hope
to solve for ϕ.

Unfortunately, it doesn't work at all

$u(r)$ is molecular potential

Nominally $\to \infty$ at $r = 0$

So for any given r, $\int |\phi(r')|^2 \, u((r-r')) \, d^3r' \to \infty$
  unless $|\phi|^2 = 0$ everywhere

Problem is that our guess for Ψ was bad.
  When two atoms are close together, $\Psi(r_1, r_2) \neq \phi(r_1)\phi(r_2)$
                                            waves are modified.

Can we save this? Yes!

Use technique call pseudopotential

For cold atoms, all collisional properties set
  by s-wave phase shift δ_0

Conventional to use scattering length $a = -\dfrac{\delta_0}{k} = -f(0)$

Get by solving radial Sch eqn for $u(r)$, as
  we discussed before.

But once we have it, we can tinker with potential
  as long as we keep the same a

In particular, replace $u \to \bar{u} = \dfrac{4\pi \hbar^2 a}{m} \, \delta^3(\vec{r})$

Then Born approx gives

$$f(\theta) = - \frac{\bar{m}}{2\pi\hbar^2} \int e^{i\vec{\kappa}\cdot\vec{r}} \cdot \frac{4\pi\hbar^2 a}{m} \delta^3(\vec{r}) d^3r = -a$$

Here $\bar{m}$ = reduced mass = $\frac{m}{2}$

So use this in our variational equation
- Correctly accounts for true pair interactions

Then

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V - \mu\right)\phi + (N-1)\phi \underbrace{\int |\phi(r')|^2 \frac{4\pi\hbar^2 a}{m} \delta^3(\vec{r}-\vec{r}') d^3r'}_{\frac{4\pi\hbar^2 a}{m}|\phi(r)|^2} = 0$$

$$\searrow \quad \simeq N \text{ if } N \gg 1$$

Or $\boxed{-\frac{\hbar^2}{2m}\nabla^2\phi + V(r)\phi + \frac{4\pi\hbar^2 a}{m}N|\phi|^2\phi = \mu\phi}$

Call nonlinear Schr. Eqn.

Correctly describes behavior of condensate

Note $N|\phi|^2$ = density of atoms
Get a "potential" term proportional to density
makes some sense.

Can solve easily in one limit : large N, $a > 0$

Then interaction potential is large and
repulsive .. tends to push atoms out
to larger r.

Then $V(r)$ term typically grows too, if U increases with r