Ground state of a quantum system of identical boson particles

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Departing from the Energy of a quantum system of identical boson particles, the field equation is derived. This is the Gross-Pitaevskii equation (GPE). A continuity equation for this system is also derived, showing that the velocity flow satisfies $\nabla \times \vec{v} = 0$, i.e.: is irrotational.

The Gross-Pitaevskii equation

Problem: derive the field equation describing the ground state of a quantum system of identical particles (bosons), that is, the Gross-Pitaevskii equation (GPE).

Background: The Gross-Pitaevskii equation is particularly useful to describe Bose Einstein condensates (BEC) of cold atomic gases [3, 4, 5], that is, an ensemble of identical quantum boson particles that interact with each other with an interaction constant G. The temperature of these cold atomic gases is typically in the ~100 nano-Kelvin range. The atom-atom interactions are repulsive for $G > 0$ and attractive for $G < 0$ (which could lead to some instabilities). The GPE is also widely used in non-linear optics to model the propagation of light in optical fibers. In this area, GPE is known as "non-linear Schrödinger equation", and the non-linearity comes from the Kerr effect [6].

Solution

One can derive this field equation the usual way, in two steps:

- Construct the Lagrangian for the system, and with it write the action functional
- The Gross-Pitaevskii equation is obtained minimizing this action, i.e., equating to zero its functional derivative with respect to the boson field.

Derivation: The system is assumed to be at sufficiently low temperature such that the particles all share the same quantum ground state $\frac{\psi}{\sqrt{N}}$, where psi is the particle-field function and N is the total particle number: $\langle \psi \mid \psi \rangle = N$. To construct the Lagrangian we thus depart from the energy density E for a quantum system of identical boson particles.

The version of Physics used is from November/26 (or later), available at the [Maplesoft Physics Research & Development webpage]

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> restart; with(Physics) : with(Physics[Vectors]) :
> interface(imaginaryunit = i) :
> Setup(mathematicalnotation = true)
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(1.1.1)

$$[\mathit{mathematicalnotation} = \mathit{true}] \tag{1.1.1}$$

Use a macro Psi = psi(x, y, z, t) to avoid redundant typing and use declare to have a compact display

> $\mathit{macro}(\mathrm{Psi} = \mathrm{psi}(x, y, z, t))$:

> $\mathit{PDEtools}{:}\text{-}\mathit{declare}((\psi, V)(x, y, z, t))$

$$\psi(x, y, z, t) \textit{ will now be displayed as } \psi$$

$$V(x, y, z, t) \textit{ will now be displayed as } V \tag{1.1.2}$$

The energy density E for a quantum system of identical boson particles is (see [3])

> $E := \hbar^2\, \mathit{Norm}(\%\mathit{Gradient}(\mathrm{Psi}))^2 / (2\, m) + V(x, y, z, t)\, \mathrm{abs}(\mathrm{Psi})^2 + (1/2)\, G\, \mathrm{abs}(\mathrm{Psi})^4;$

$$E := \frac{\hbar^2\, \|\nabla\psi\|^2}{2\, m} + V\, |\psi|^2 + \frac{G\, |\psi|^4}{2} \tag{1.1.3}$$

where $\hbar$ is the Planck constant divided by $2 \cdot \pi$, m the mass of a single particle, psi(x, y, z, t) a complex field, $V(x, y, z, t)$ an arbitrary external potential and the interaction term G takes into account atom-atom interactions. So set the real objects for this problem

> $\mathit{Setup}(\mathit{realobjects} = \{t, m, \hbar, G, V(x, y, z, t)\})$

$$[\mathit{realobjects} = \{\hbar, G, \hat{i}, \hat{j}, \hat{k}, \hat{\phi}, \hat{r}, \hat{\rho}, \hat{\theta}, m, \phi, r, \rho, t, \theta, x, y, z, V\}] \tag{1.1.4}$$

The Lagrangian density L is defined in terms of the Energy E in the usual way

> $L := \left(\frac{i\, \hbar}{2}\right) (\mathit{conjugate}(\mathrm{Psi})\, \mathit{diff}(\mathrm{Psi}, t) - \mathrm{Psi} * \mathit{diff}(\mathit{conjugate}(\mathrm{Psi}), t)) - E$

$$L := \frac{\mathrm{i}\, \hbar\, (\overline{\psi}\, \psi_t - \psi\, \overline{\psi}_t)}{2} - \frac{\hbar^2\, \|\nabla\psi\|^2}{2\, m} - V\, |\psi|^2 - \frac{G\, |\psi|^4}{2} \tag{1.1.5}$$

The corresponding Action S

> $S := \mathit{Intc}(L, x, y, z, t)$

$$S := \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\frac{\mathrm{i}\, \hbar\, (\overline{\psi}\, \psi_t - \psi\, \overline{\psi}_t)}{2} - \frac{\hbar^2\, \|\nabla\psi\|^2}{2\, m} - V\, |\psi|^2 - \frac{G\, |\psi|^4}{2}\right) \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}t \tag{1.1.6}$$

Minimizing the action gives the field equations, so taking the functional derivative

> $S, \psi(X, Y, Z, T)$:
> $\mathit{subs}(\{X = x, Y = y, Z = z, T = t\}, (\%\mathit{Fundiff} = \mathit{Fundiff})(\%))$

$$\left(\frac{\delta}{\delta\psi}\right) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\frac{\mathrm{i}\, \hbar\, (\overline{\psi}\, \psi_t - \psi\, \overline{\psi}_t)}{2} - \frac{\hbar^2\, \|\nabla\psi\|^2}{2\, m} - V\, |\psi|^2 - \frac{G\, |\psi|^4}{2}\right) \mathrm{d}x\, \mathrm{d}y\, \mathrm{d}z\, \mathrm{d}t = \frac{\hbar^2\, \overline{\psi}_{x,x} + \overline{\psi}_{y,y}\, \hbar^2 + \hbar^2\, \overline{\psi}_{z,z} - 2\, (G\, \overline{\psi}^2\, \psi + \mathrm{i}\, \overline{\psi}_t\, \hbar + \overline{\psi}\, V)\, m}{2\, m} \tag{1.1.7}$$

Equating this result to 0 is the desired field equation, GPE. This result can be compacted to arrive at the standard form of the GPE. For instance, in the right-hand side of **(1.1.7)** we see a Laplacian in disguise. So take the conjugate and isolate the time derivative:

> $\mathit{conjugate}(\mathit{rhs}(\textbf{(1.1.7)}) = 0)$

$$\frac{\frac{\hbar^2 \psi_{x,x}}{2} + \frac{\psi_{y,y}\hbar^2}{2} + \frac{\hbar^2 \psi_{z,z}}{2} - \frac{m\left(-2\,\mathrm{i}\,\psi_t \hbar + 2\,\psi V + 2\,G\,\psi^2\,\overline{\psi}\right)}{2}}{m} = 0 \qquad \textbf{(1.1.8)}$$

> $i\,\hbar\;isolate(\textbf{(1.1.8)}, diff(\mathrm{Psi}, t))$

$$\mathrm{i}\,\psi_t\,\hbar = \frac{-\frac{\hbar^2 \psi_{x,x}}{2} - \frac{\psi_{y,y}\hbar^2}{2} - \frac{\hbar^2 \psi_{z,z}}{2}}{m} + \psi V + G\,\psi^2\,\overline{\psi} \qquad \textbf{(1.1.9)}$$

Introduce in **(1.1.9)** the Laplacian

> $(Laplacian = \%Laplacian)(\mathrm{Psi})$

$$\psi_{x,x} + \psi_{y,y} + \psi_{z,z} = \nabla^2\psi \qquad \textbf{(1.1.10)}$$

> $algsubs(\textbf{(1.1.10)}, \textbf{(1.1.9)})$

$$\mathrm{i}\,\psi_t\,\hbar = -\frac{\hbar^2\,\nabla^2\psi}{2\,m} + G\,\psi^2\,\overline{\psi} + \psi V \qquad \textbf{(1.1.11)}$$

The product psi $\overline{\text{psi}}$ can be rewritten as |psi| and, collecting psi, we arrive at the standard form of the Gross–Pitaevskii equation

> $collect(convert(\textbf{(1.1.11)}, \mathrm{abs}), \mathrm{psi})$

$$\mathrm{i}\,\psi_t\,\hbar = \left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m} \qquad \textbf{(1.1.12)}$$

So the GPE looks like the usual Schrödinger equation, except there is a non-linear term acting as a potential proportional to the local field intensity $|\psi|^2$.

Continuity equation for a quantum system of identical particles

Like for the standard Schrödinger equation, it is possible to derive a continuity equation for the ground state of a quantum system of identical particles that is similar to the one in fluid mechanics. Because the non linear term $G\,|\psi|^2$ is real, the continuity equation will be independent of this non linearity (and of the potential V as well).

To obtain the continuity equation, GPE **(1.1.12)** is first multiplied by $\overline{\psi}$; then the complex conjugate of the resulting product is subtracted:

> $conjugate(\mathrm{Psi})\;\textbf{(1.1.12)}$

$$\mathrm{i}\,\hbar\,\overline{\psi}\,\psi_t = \overline{\psi}\left(\left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m}\right) \qquad \textbf{(2.1)}$$

> $\textbf{(2.1)} - conjugate(\textbf{(2.1)})$

$$\mathrm{i}\,\hbar\,\overline{\psi}\,\psi_t + \mathrm{i}\,\hbar\,\psi\,\overline{\psi}_t = \overline{\psi}\left(\left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m}\right) - \psi\,\overline{\left(\left(G\,|\psi|^2 + V\right)\psi - \frac{\hbar^2\,\nabla^2\psi}{2\,m}\right)} \qquad \textbf{(2.2)}$$

> $expand\left(\frac{\textbf{(2.2)}}{\mathrm{i}\cdot\hbar}\right)$

$$\overline{\psi}\,\psi_t + \psi\,\overline{\psi}_t = \frac{\mathrm{i}\,\hbar\,\overline{\psi}\,\nabla^2\psi}{2\,m} - \frac{\mathrm{i}\,\hbar\,\psi\,\nabla^2\overline{\psi}}{2\,m} \tag{2.3}$$

The left hand side of **(2.3)** can be integrated, consider

> $\%diff\left(\mathrm{abs}(\mathrm{Psi})^2, t\right)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) \tag{2.4}$$

> $convert(\textbf{(2.4)}, conjugate) = \textbf{(2.4)}$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\psi\,\overline{\psi}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) \tag{2.5}$$

> $value(lhs(\textbf{(2.5)})) = rhs(\textbf{(2.5)})$

$$\overline{\psi}\,\psi_t + \psi\,\overline{\psi}_t = \frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) \tag{2.6}$$

So **(2.3)** becomes

> $subs(\textbf{(2.6)}, \textbf{(2.3)})$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) = \frac{\mathrm{i}\,\hbar\,\overline{\psi}\,\nabla^2\psi}{2\,m} - \frac{\mathrm{i}\,\hbar\,\psi\,\nabla^2\overline{\psi}}{2\,m} \tag{2.7}$$

The right-hand side of this result can also be rewritten as a divergence, consider

> $conjugate(\mathrm{Psi})\ \%Gradient(\mathrm{Psi}) - \mathrm{Psi}\ \%Gradient(conjugate(\mathrm{Psi}))$

$$\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi} \tag{2.8}$$

Take now the divergence and compare with its expanded form

> $(\%Divergence = expand@\%Divergence)(\textbf{(2.8)})$

$$\nabla\cdot\left(\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi}\right) = \overline{\psi}\,\nabla^2\psi - \psi\,\nabla^2\overline{\psi} \tag{2.9}$$

Multiply by the proper factors of the right-hand side of **(2.7)**

> $\dfrac{\mathrm{i}\,\hbar\,\textbf{(2.9)}}{2\,m}$

$$\frac{\frac{\mathrm{i}}{2}\,\hbar\,\nabla\cdot\left(\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi}\right)}{m} = \frac{\frac{\mathrm{i}}{2}\,\hbar\left(\overline{\psi}\,\nabla^2\psi - \psi\,\nabla^2\overline{\psi}\right)}{m} \tag{2.10}$$

The right-hand side of this result is equal to the right-hand side of **(2.7)** . So subtract this result and isolate the time derivative $\frac{\partial}{\partial t}\,|\mathrm{psi}|^2$

> $normal(\textbf{(2.7)} - \textbf{(2.10)})$

$$-\frac{\mathrm{i}\,\hbar\,\nabla\cdot\left(\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi}\right) - 2\,\frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right)m}{2\,m} = 0 \tag{2.11}$$

> $isolate\left(\textbf{(2.11)}, \%diff\left(\mathrm{abs}(\mathrm{Psi})^2, t\right)\right)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) = \frac{\frac{\mathrm{i}}{2}\,\hbar\,\nabla\cdot\left(\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi}\right)}{m} \tag{2.12}$$

To express **(2.12)** as a typical continuity equation, the argument of the divergence operator can be rewritten as the product of the particle density $n(x, y, z, t)$ times a velocity field $\vec{v}(x, y, z, t)$, where the density satisfies $n(x, y, z, t) = |\psi|^2 \geq 0$.

> *PDEtools:-declare*$((n, v\_)(x, y, z, t))$

$$n(x, y, z, t) \text{ will now be displayed as } n$$
$$\vec{v}(x, y, z, t) \text{ will now be displayed as } \vec{v} \tag{2.13}$$

> *Setup*$(realobjects = n(x, y, z, t))$

$$[realobjects = \{\hbar, G, \hat{i}, \hat{j}, \hat{k}, \hat{\phi}, \hat{r}, \hat{\rho}, \hat{\theta}, m, \phi, r, \rho, t, \theta, x, y, z, V, n\}] \tag{2.14}$$

So the argument of the divergence $\nabla\cdot\left(\overline{\text{psi}}\,(\nabla \text{psi}) - \text{psi}\,(\nabla \overline{\text{psi}})\right)$ **(2.12)** can be expressed as

> $op(op(3, rhs(\textbf{(2.12)}))) = \text{abs}(\text{Psi})^2\, v\_(x, y, z, t) \left(\frac{2\, m\, i}{\hbar}\right)$

$$\overline{\psi}\,\nabla\psi - \psi\,\nabla\overline{\psi} = \frac{2\,\mathrm{i}\,|\psi|^2\,\vec{v}\,m}{\hbar} \tag{2.15}$$

> *subs*$(\textbf{(2.15)}, \textbf{(2.12)})$

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(|\psi|^2\right) = \frac{\frac{\mathrm{i}}{2}\,\hbar\,\nabla\cdot\left(\frac{2\,\mathrm{i}\,|\psi|^2\,\vec{v}\,m}{\hbar}\right)}{m} \tag{2.16}$$

Introducing now the particle density *n and expanding*

> $\text{abs}(\text{Psi})^2 = n(x, y, z, t)$

$$|\psi|^2 = n \tag{2.17}$$

> *subs*$(\textbf{(2.17)}, \textbf{(2.16)})$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,n = \frac{\frac{\mathrm{i}}{2}\,\hbar\,\nabla\cdot\left(\frac{2\,\mathrm{i}\,n\,\vec{v}\,m}{\hbar}\right)}{m} \tag{2.18}$$

> $lhs(\textbf{(2.18)}) = expand(rhs(\textbf{(2.18)}))$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,n = -n\,\nabla\cdot\vec{v} - \nabla n\cdot\vec{v} \tag{2.19}$$

That is,

> $lhs(\textbf{(2.19)}) = -\ \%Nabla((n\ v\_)(x, y, z, t))$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,n = -\nabla\,(n\,\vec{v}) \tag{2.20}$$

One can still verify that, provided that there are no singularities, i.e. $n \neq 0$, the velocity satisfies $\nabla\times\vec{v} = 0$, it can be written as a gradient, $\vec{v} = \frac{\hbar}{m}\nabla s$. That is, GPE admits solutions with vortices. At the center of a vortex, the field density vanishes, $n = 0$. This singularity warrants that the velocity circulation around a vortex is not 0 (indeed, it is quantified, but that is beyond the scope of this worksheet).

To verify that $\nabla\times\vec{v} = 0$, ψ is rewritten as a function of its phase s (so s is real) and amplitude $\sqrt{n}$,

> *PDEtools:-declare*$(s(x, y, z, t))$

$$s(x, y, z, t) \text{ will now be displayed as } s \tag{2.21}$$

> $Setup(realobjects = s(x, y, z, t))$

$$\left[realobjects = \{\hbar, G, \hat{i}, \hat{j}, \hat{k}, \hat{\phi}, \hat{r}, \hat{\rho}, \hat{\theta}, m, \phi, r, \rho, t, \theta, x, y, z, V, n, s\}\right] \tag{2.22}$$

> $\mathrm{Psi} = \mathrm{sqrt}(n(x, y, z, t))\, e^{I\, s(x, y, z, t)}$

$$\psi = \sqrt{n}\, e^{i s} \tag{2.23}$$

Substituting this value in **(2.15)**

> $eval(\textbf{(2.15)}, \textbf{(2.23)})$

$$\frac{\sqrt{n}\, \nabla\left(\sqrt{n}\, e^{i s}\right)}{e^{i s}} - \sqrt{n}\, e^{i s}\, \nabla\left(\frac{\sqrt{n}}{e^{i s}}\right) = \frac{2\, i\, |n|\, \vec{v}\, m}{\hbar} \tag{2.24}$$

Taking into account that outside the center of the vortex $n > 0$ and isolating the velocity $\vec{v}$

> $simplify(\textbf{(2.24)})$ assuming $n(x, y, z, t) > 0$

$$n\left(e^{-i s}\, \nabla e^{i s} - e^{i s}\, \nabla e^{-i s}\right) = \frac{2\, i\, n\, \vec{v}\, m}{\hbar} \tag{2.25}$$

> $isolate(\textbf{(2.25)}, v\_(x, y, z, t))$

$$\vec{v} = \frac{-\frac{i}{2}\left(e^{-i s}\, \nabla e^{i s} - e^{i s}\, \nabla e^{-i s}\right) \hbar}{m} \tag{2.26}$$

The right hand side can now be conveniently rewritten as a gradient. For that purpose, compute first the inert gradient functions of **(2.26)**

> $expand(value(\textbf{(2.26)}))$

$$\vec{v} = \frac{\hbar\, s_x\, \hat{i}}{m} + \frac{\hbar\, s_y\, \hat{j}}{m} + \frac{\hbar\, s_z\, \hat{k}}{m} \tag{2.27}$$

This result can recombined as a gradient of the phase $s(x, y, z, t)$

> $(Gradient = \%Gradient)(s(x, y, z, t))$

$$s_x\, \hat{i} + s_y\, \hat{j} + s_z\, \hat{k} = \nabla s \tag{2.28}$$

> $algsubs(\textbf{(2.28)}, \textbf{(2.27)})$

$$\vec{v} = \frac{\hbar\, \nabla s}{m} \tag{2.29}$$

And from this result it follows that

> $Curl(\textbf{(2.29)})$

$$\nabla \times \vec{v} = 0 \tag{2.30}$$

The continuity equation **(2.18)** can finally be rewritten, now carrying the information about $\nabla \times \vec{v} = 0$, directly in terms of $s(x, y, z, t)$ as

> $subs(\textbf{(2.29)}, \textbf{(2.20)})$

$$\frac{d}{dt}\, n = -\nabla\left(\frac{n\, \hbar\, \nabla s}{m}\right) \tag{2.31}$$

or in expanded form

> $expand(\textbf{(2.31)})$

(2.32)

$$\frac{d}{dt} n = -\frac{n \hbar \nabla^2 s}{m} - \frac{\hbar (\nabla n \cdot \nabla s)}{m} \quad \textbf{(2.32)}$$

References

[1] Gross-Pitaevskii equation (wiki)
[2] Continuity equation (wiki)
[3] Bose–Einstein condensate (wiki)
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