Mean field approach; Self-consistent - Response

Computational Physics

4. október 2010

We have a finite electron system in an external potential

$$\phi_{\text{ext}} = \phi_0 e^{-i(\omega+i\eta)t}$$

The total electrostatic potential is

$$\phi_{\text{sc}}(\mathbf{r},t) = \phi_{\text{ext}}(\mathbf{r},t) + \phi_{\text{ind}}(\mathbf{r},t)$$

where ϕ_{ext} is caused by the change in the charge distribution

$$\phi_{\text{ind}}(\mathbf{r},t) = -\frac{e}{\kappa}\int d\mathbf{r}'\frac{\delta n(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}$$

and the density variation $\delta n(\mathbf{r},t)$ is caused by the total electrostatic potential $\phi_{\text{sc}}(\mathbf{r},t)$

$$\delta n(\mathbf{r},t) = \int d\mathbf{r}' \chi(\mathbf{r},\mathbf{r}',t)(-e\phi_{\rm sc}(\mathbf{r}',t))$$

So we can have a self-consistent equation for $\phi_{\rm sc}$

$$\phi_{\rm sc}(\mathbf{r},t) = \phi_{\rm ext}(\mathbf{r},t) + \frac{e^2}{\kappa}\int d\mathbf{r}' d\mathbf{r}'' \, \frac{\chi(\mathbf{r}',\mathbf{r}'',t)}{|\mathbf{r}-\mathbf{r}'|}\phi_{\rm sc}(\mathbf{r}'',t)$$

which is an integral equation in real space. It can be put on a grid and transformed into a matrix equation, but it is more effective to fourier transform it first

$$\phi_{\rm sc}(\mathbf{k},\omega) = \phi_{\rm ext}(\mathbf{k},\omega) + \frac{4\pi e^2}{\kappa k^2}\int d\mathbf{q} \, \chi(\mathbf{k},\mathbf{q},\omega)\phi_{\rm sc}(\mathbf{q},\omega) \quad (*)$$

where a convolution property of the Coulomb kernel was used

and the fourier transform of the response function

$$\chi(\mathbf{k},\mathbf{q},\omega) = \frac{1}{(2\pi)^3}\int d\mathbf{r}\, d\mathbf{r}' e^{-i\mathbf{k}\cdot\mathbf{r}}\chi(\mathbf{r},\mathbf{r}',\omega)e^{i\mathbf{q}\cdot\mathbf{r}'}$$

As $(*)$ connects the external and the total electrostatic potential we can compare it to $\mathbf{D} = \epsilon\mathbf{E}$ to write for the dielectric function

$$\epsilon(\mathbf{k},\mathbf{q},\omega) = \delta(\mathbf{k}-\mathbf{q}) - \frac{4\pi e^2}{\kappa k^2}\chi(\mathbf{k},\mathbf{q},\omega)$$

for a 3D finite electron system, in a 2D system the fourier transform of the Coulomb kernel is different.

Numerical evaluation

Equation $(*)$ is an integral equation, one way to solve it is on a **q**-grid. (specially convenient if some symmetry can be used to reduce the spatial dimensions).

Grid transforms it to a matrix equation

$$\phi_{\rm sc} = \phi_{\rm ext} + G\chi\phi_{\rm sc} \quad \text{or} \quad (1 - G\chi)\phi_{\rm sc} = \phi_{\rm ext}$$

which is equivalent to

$$\epsilon\phi_{\rm sc} = \phi_{\rm ext} \quad \text{or} \quad \phi_{\rm sc} = (1 - G\chi)^{-1}\phi_{\rm ext} = \epsilon^{-1}\phi_{\rm ext}$$

The matrix expression

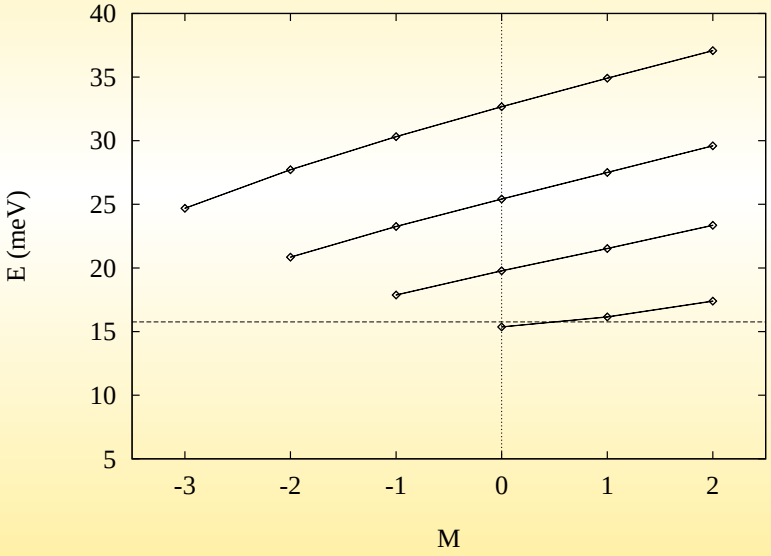
$$\phi_{\rm sc}(\omega) = (1 - G\chi(\omega))^{-1}\phi_{\rm ext}(\omega) = \epsilon^{-1}(\omega)\phi_{\rm ext}(\omega)$$

- tells us that zeros in $\epsilon(\omega)$ or poles in $\epsilon^{-1}(\omega)$ mean that small external perturbation $\phi_{\rm ext}(\omega)$ could cause a huge total potential $\phi_{\rm sc}(\omega) \rightarrow$ a resonance.
- A small perturbation might cause an oscillation of the charge density $\rightarrow$ plasma waves, plasmons.
- The plasmon would not happen at any of the Bohr frequencies $\omega_\alpha - \omega_\beta$, it is a collective mode with a depolarization shift.
- In a system with a size much smaller than the wavelength of an external EM radiation $\phi_{\rm ext}(\omega)$ can describe this radiation $\rightarrow$ we can calculate the resonance frequencies at which the system absorbs energy.

Example

Two electrons in a 2D parabolic quantum dot in a magnetic field B. HA.

$B = 1$ T, both occupy the $(n_r, M) = (0, 0)$ state, but with opposite spin.



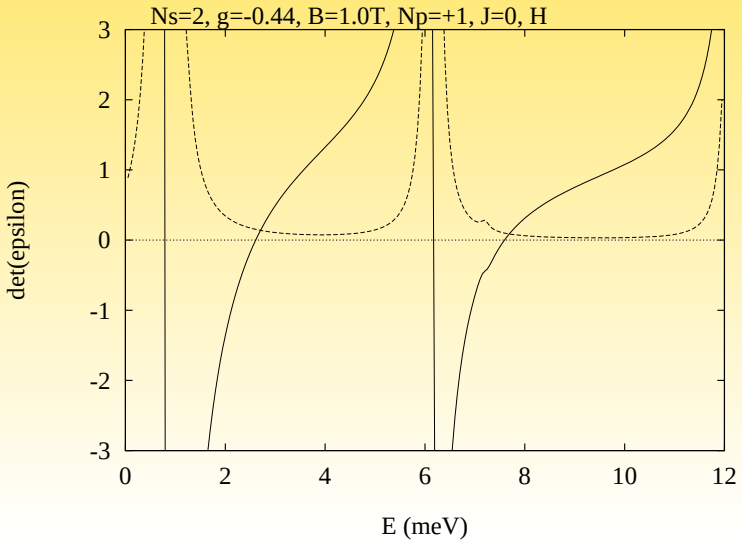
Angular symmetry → here we use a q-grid and expand the angular dependence analytically in $\exp(-iN_p\phi)$ terms with $N_p = 0, \pm 1, \pm 2 \ldots$.

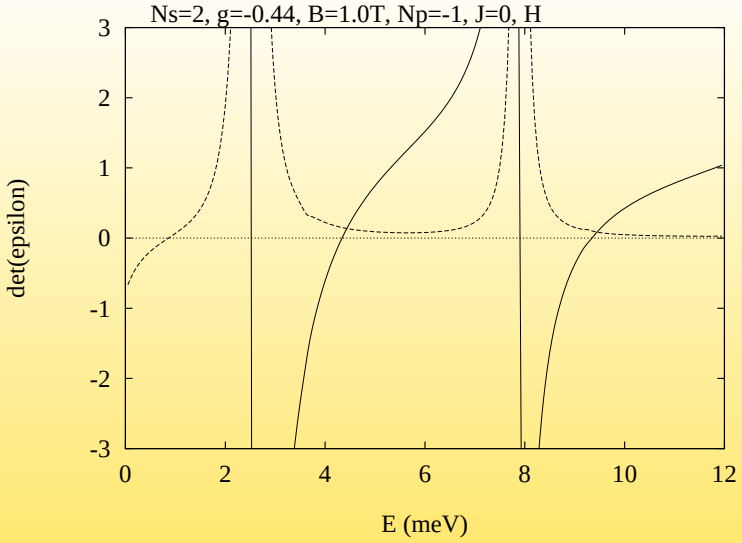
Multipole expansion

Graph $\det \epsilon(\omega)$

Single-electron energy levels → large imaginary part

Collective oscillations → almost a complex zero, (η is finite).

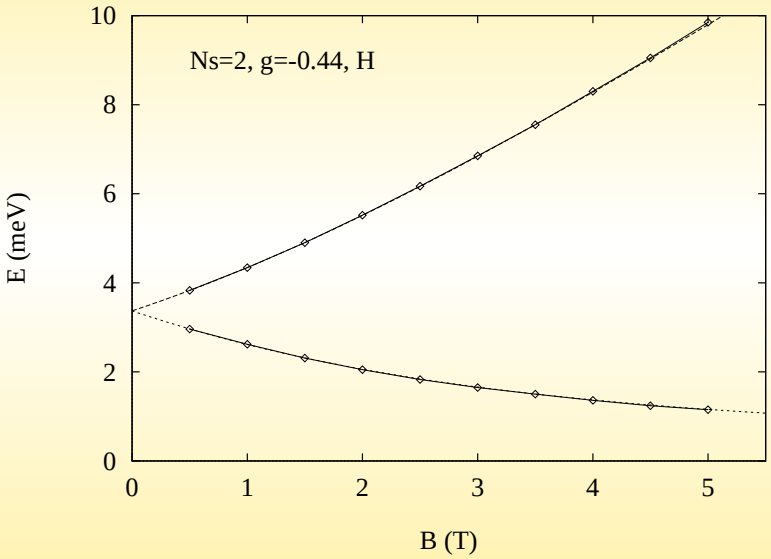




The dispersion of the collective dipole mode $N_P = \pm 1$

Agrees with an exact analytic calculation, only center-of-mass mode is excited. This is not used in the program.

Higher order modes.



The search for zeros in $\det \epsilon(\omega)$ is very complicated in larger systems. Better to use the symmetry of the external field in an absorption formula. η is kept finite but small $\rightarrow$ power dissipation, heating.
Use the Joule heating

$$P(\omega) = \frac{1}{2} \int d\mathbf{r} \Re[\mathbf{j}(\mathbf{r}) \cdot \mathbf{E}^*(\mathbf{r})]$$

In a 2D system the connection between the response function and the conductivity

$$-\frac{e^2}{\kappa} \chi^{2D}(\mathbf{k}, \mathbf{q}, \omega) = \frac{i}{\omega} \mathbf{k} \cdot \sigma(\mathbf{k}, \mathbf{q}, \omega) \cdot \mathbf{q}$$

gives

$$P(\omega) = -\frac{1}{2} \frac{\omega}{(2\pi)^3} \int d\mathbf{k} \Im[k \phi_{\mathrm{sc}}(\mathbf{k}, \omega) \phi^*_{\mathrm{ext}}(\mathbf{k}, \omega)]$$

If $n(\mathbf{r},t)$ is not a primary variable

We use the HFA as an example

$$\hat{H}(t) = \hat{H}_{HF} + \delta\hat{V}e^{-i(\omega+i0^+)t}$$

Linear response, ($\{\ |\alpha\rangle\}$ are the eigen states of H_{HF})

$$\delta\rho_{\alpha,\beta}(t) = f^{\alpha,\beta}(\omega)\langle\alpha|\delta\hat{V}|\beta\rangle e^{-i(\omega+i0^+)t}$$

with

$$f^{\alpha,\beta}(\omega) = \left\{\frac{f(\epsilon_\beta) - f(\epsilon_\alpha)}{\hbar\omega + (\epsilon_\beta - \epsilon_\alpha) + i\hbar 0^+}\right\}$$

Nonlocal exchange

$$\delta V_{\alpha,\beta} = (-e)\left\{\langle\alpha|\phi_{\rm ext}|\beta\rangle + \langle\alpha|\phi^H_{\rm ind}|\beta\rangle + \langle\alpha|\phi^F_{\rm ind}|\beta\rangle\right\}$$

Self-consistence $\longleftarrow$ $\langle\alpha|\phi^{H,F}_{\rm ind}|\beta\rangle \sim \delta\rho_{\alpha,\beta}$.

Leads to

$$\sum_{\delta,\gamma} \epsilon_{\alpha\beta,\delta\gamma}(\omega)\langle\delta|\phi_{sc}|\gamma\rangle = \langle\alpha|\phi_{ext}|\beta\rangle$$

with

$$\epsilon_{\alpha\beta,\delta\gamma}(\omega) = \left\{\delta_{\delta,\alpha}\delta_{\gamma,\beta} - \left(H_{\gamma\delta,\beta\alpha} - F_{\gamma\delta,\beta\alpha}\right) f^{\delta\gamma}(\omega)\right\}$$

$$H_{\gamma\delta,\beta\alpha} = \frac{e^2}{\kappa}\int d\mathbf{r}d\mathbf{r}' \, \frac{\psi^*_\gamma(\mathbf{r}')\psi_\delta(\mathbf{r}')\psi^*_\alpha(\mathbf{r})\psi_\beta(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$$

$$F_{\gamma\delta,\beta\alpha} = \frac{e^2}{\kappa}\int d\mathbf{r}d\mathbf{r}' \, \frac{\psi^*_\gamma(\mathbf{r}')\psi_\delta(\mathbf{r})\psi^*_\alpha(\mathbf{r}')\psi_\beta(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$$

Now one could use

$$\det \epsilon_{\alpha\beta,\delta\gamma}(\omega) = 0, \qquad \alpha = (n, M, s) \quad \text{for a 2D quantum dot}$$

or calculate the absorption

$$P(\omega) = \frac{1}{2}\int d\mathbf{r}\ \mathrm{Re}\left[\delta\mathbf{j}(\mathbf{r})\cdot\mathbf{E}^{*}_{sc}(\mathbf{r})\right]$$

which for a 2D quantum dot gives

$$P(\omega) = e\mathcal{E}^{\mathrm{ext}}\omega\sum_{\alpha\beta}\langle\beta|r^{|N_p|}|\alpha\rangle 2\pi\delta_{M_\beta,M_\alpha\pm N_p}\Im\{f^{\alpha\beta}(-e\phi^{\mathrm{sc}}_{\alpha\beta})\}$$

if the external electrostatic potential is

$$\phi^{\mathrm{ext}}(\mathbf{r},t) = \mathcal{E}^{\mathrm{ext}}r^{|N_p|}\exp\left\{-i(\omega+i0^{+})t - iN_p\varphi\right\}$$

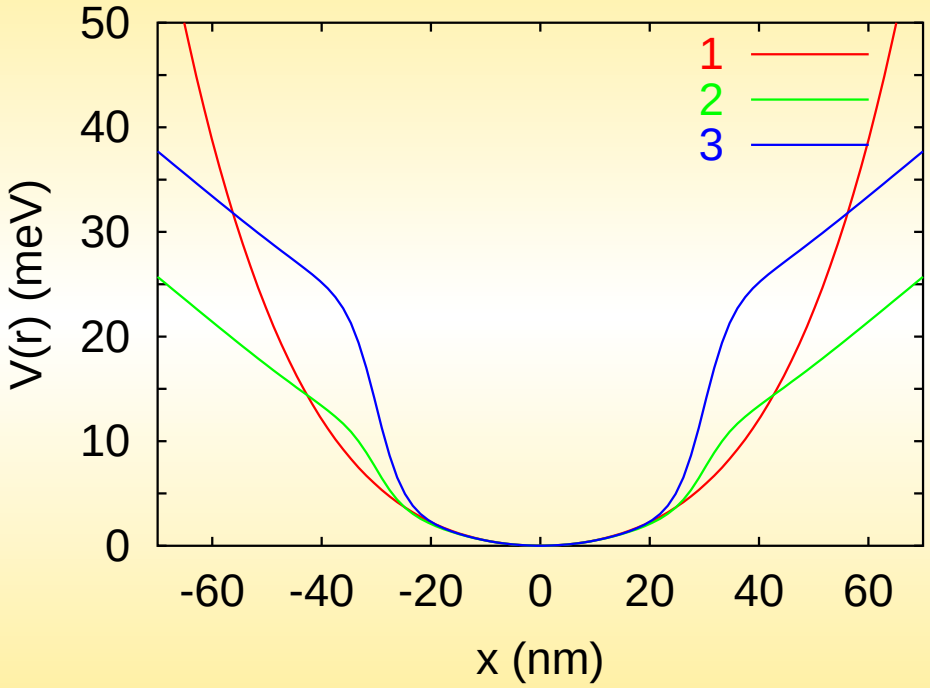
- Here the equation for ϕ^{SC} is already in a matrix form, but the number of states involved can make it quite large.
- η is used in a simplistic way to mimic the linewidth observed in experiments.
- In a real space method ($\mathbf{r}$ or $\mathbf{q}$) one can calculate $\delta(\mathbf{r}, t)$ to identify modes.
- In HFA one can not calculate directly what type of density oscillations occur, but it is possible to find out which single-electron transitions contribute the most.

Example:
dot with nonparabolic confinement

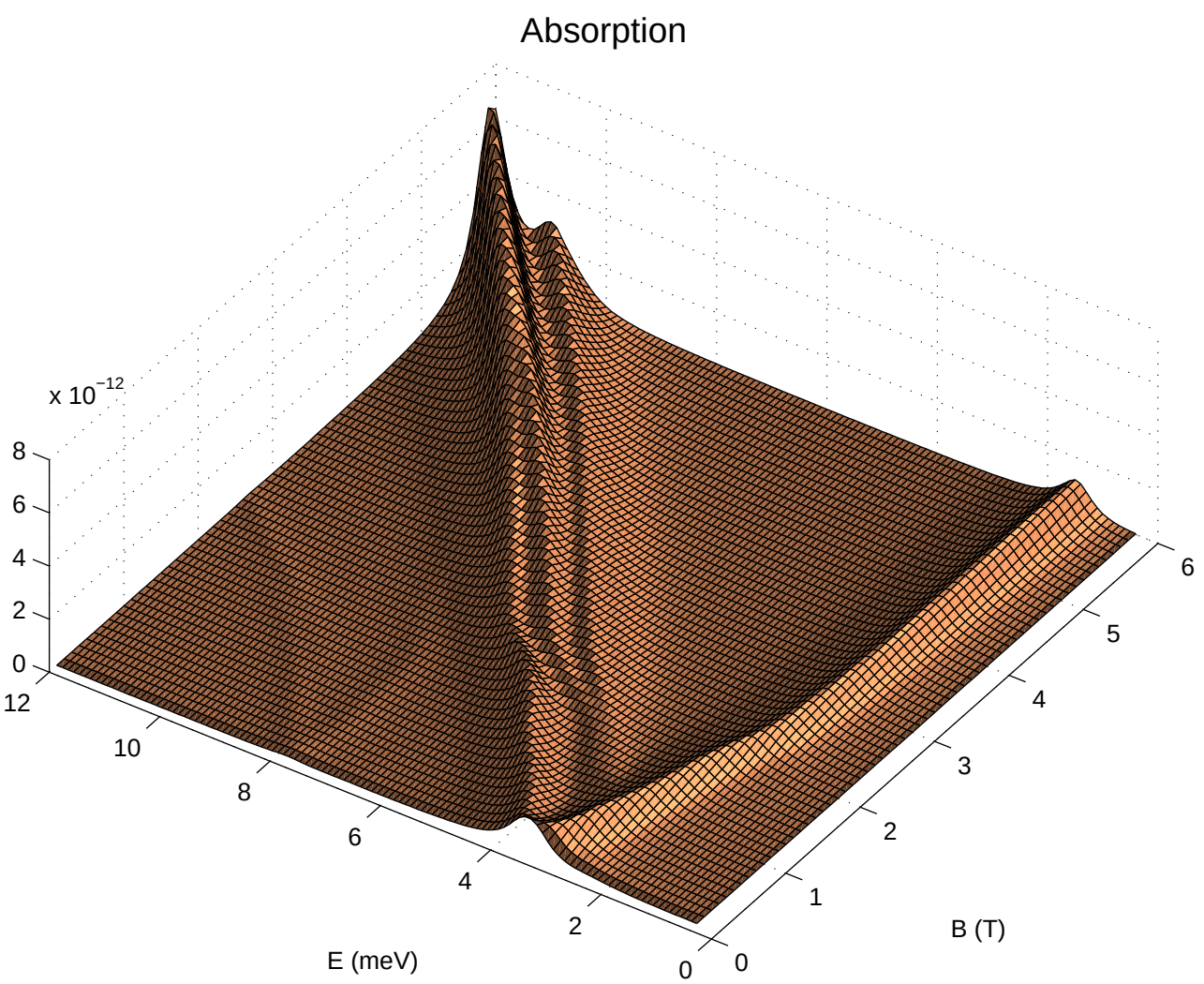
Parabolic + higher terms...

↓

excitations above the upper Kohn mode



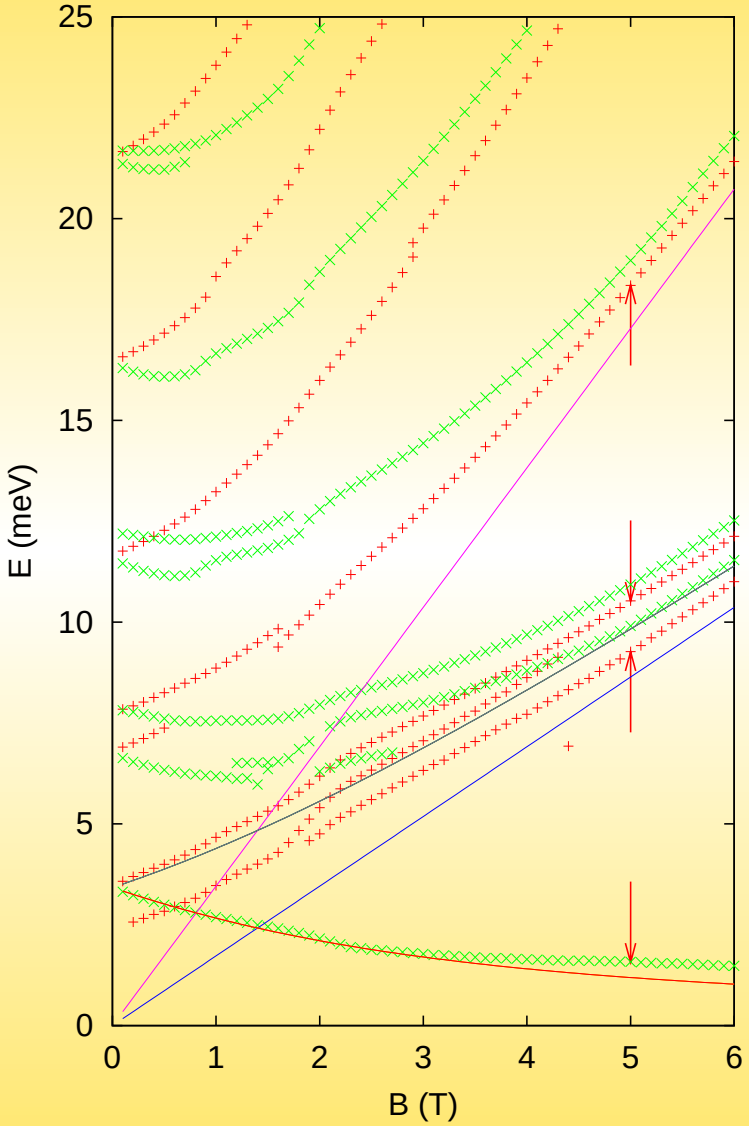
Calculated power absorption, ($N = 5$, $T = 1$ K)



Calculated dispersion

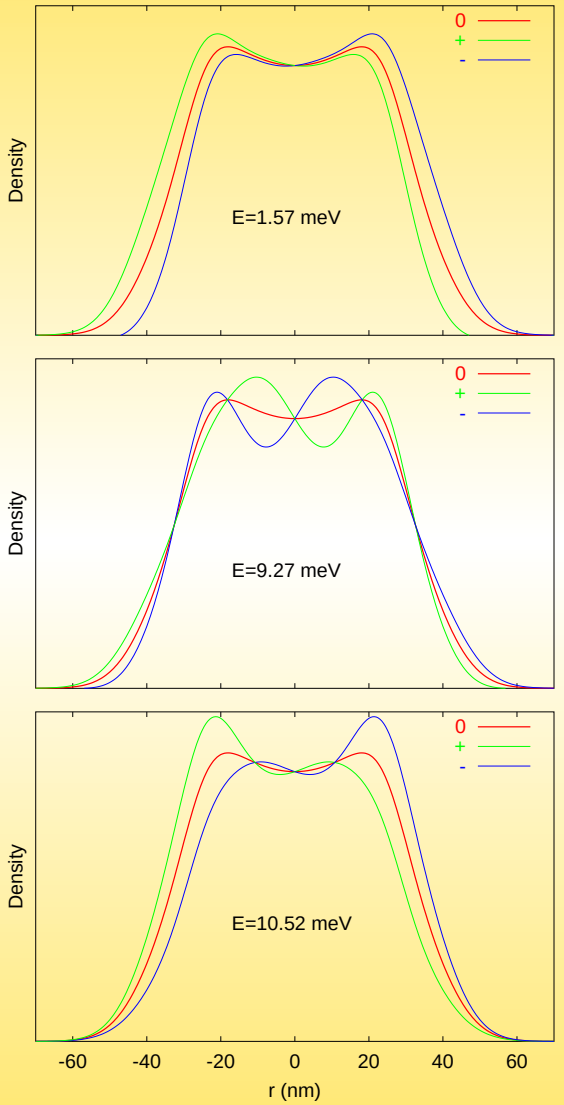
$N = 5$, $T = 1$ K

- Left, right polarization
- Bernstein modes (class.)



Induced density

- Mode recognition
- CM $\leftrightarrow$ relative motion



Many other effects can be studied combining MF and linear response. We have only take a simple example here of the density response in order to introduce computational technical points.