Mean field approach - Time-dependent - Response

Computational Physics

4. október 2010

The mean field approach has also been extended to time-dependent problems

How does a system **respond** to an external time-dependent potential?

- Real-time response, (tdHA, tdHFA or tdLDA), on a lattice, or in a basis.
- Linear response in real or fourier space, (tdHA or tdLDA), or in a basis, (tdHFA. . .).

There are many more important approaches we skip here.

Real-time response, (tdHF) A. Puente, L. Serra, and V. Gudmundsson, Phys. Rev. B 64, 235324 (2001), (cond-mat/0108428)., (Atomic units).

$$
\begin{aligned}
i\frac{\partial}{\partial t}\varphi_{i\eta}(\mathbf{r}_1,t) &= \left[\frac{(-i\nabla+\gamma\mathbf{A}(\mathbf{r}_1))^2}{2} + v_H(\mathbf{r}_1,t) + v_{\mathrm{ext}}(\mathbf{r}_1,t)\right. \\
&+ \left.\frac{1}{2}g^*m^*\gamma B s_z\right]\varphi_{i\eta}(\mathbf{r}_1,t) - \int d\mathbf{r}_2\,\frac{\rho_\eta(\mathbf{r}_2,\mathbf{r}_1,t)}{r_{12}}\,\varphi_{i\eta}(\mathbf{r}_2,t)
\end{aligned}
$$

$$
\gamma = e/c, \qquad \rho_\eta(\mathbf{r}_2,\mathbf{r}_1,t) = \sum_{i,occ.}\varphi_{i\eta}(\mathbf{r}_2,t)^*\varphi_{i\eta}(\mathbf{r}_1,t)
$$

Cranck-Nicholson algorithm

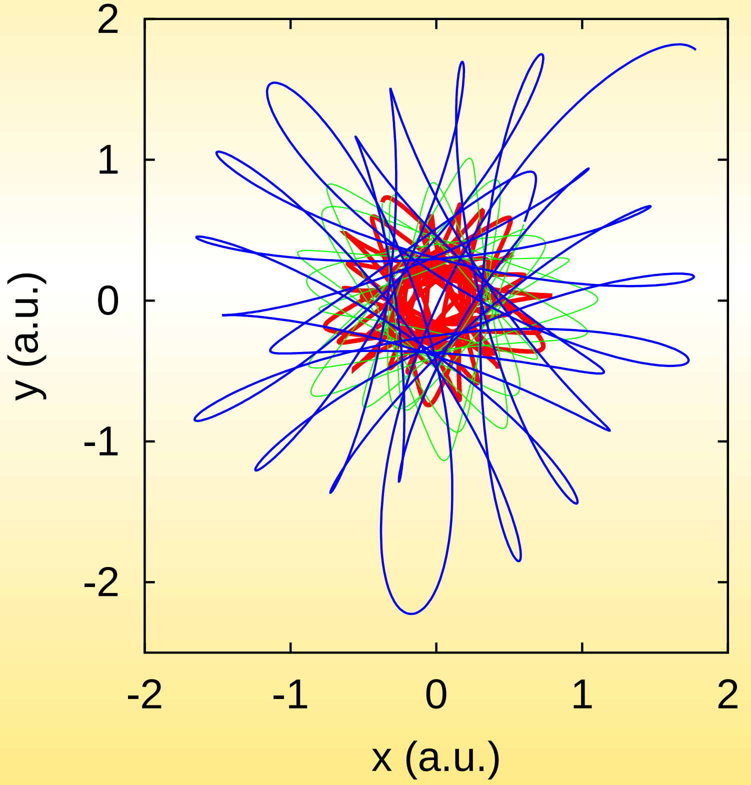
$$
\left(1+\frac{i\Delta t}{2}h_0^{(k+1)}\right)\varphi_{i\eta}^{(k+1)} = \left(1-\frac{i\Delta t}{2}h_0^{(k)}\right)\varphi_{i\eta}^{(k)} + \frac{i\Delta t}{2}\left(\mathcal{V}_{i\eta}^{(k)}+\mathcal{V}_{i\eta}^{(k+1)}\right)
$$

Initial rigid displacement $\mathbf{e}$, $\rightarrow$ analyze dipole moment $\langle\mathbf{e}\cdot\mathbf{r}\rangle_t$

Example, six electrons in a quantum dot, nonparabolic confinement, $B \neq 0$.

Motion of the center-of-mass in the tdHA

- 9000 time-steps
- 3 intervals of 12 ps
- $B = 1$ T
- Amplitude shrinks
- Total energy is constant



→ Energy must flow into internal modes

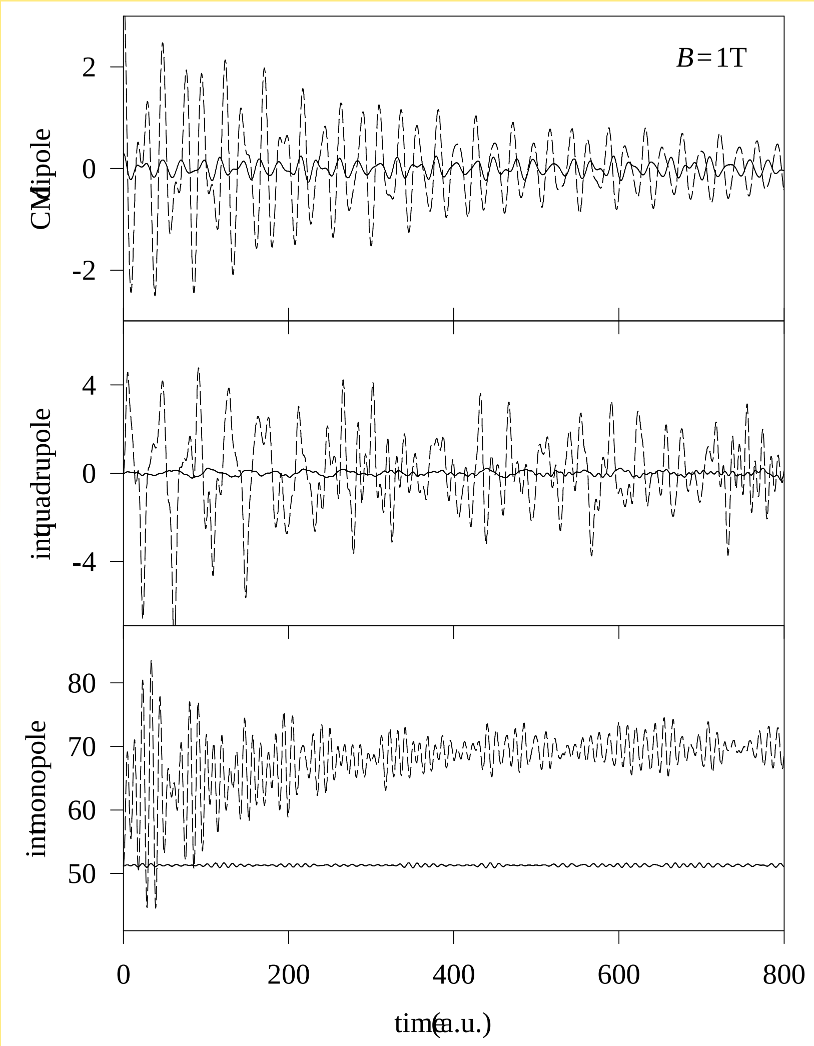
Internal Quadrupole and Monopole, (cm-frame)

$$\tilde{\mathbf{r}} = \mathbf{r} - \mathbf{R}_{cm}$$

$$\tilde{Q} = \sum_i \tilde{x}\tilde{y} = \sum_i x_i y_i - \frac{1}{N}\sum_{ik} x_i y_k$$

$$\tilde{M} = \sum_i \tilde{x}^2 + \tilde{y}^2 = \sum_i x_i^2 + y_i^2 - \frac{1}{N}\sum_{ik} x_i x_k + y_i y_k$$

Take expectations values (t-dependent).



Time evolution

- Weak amplitude
- Strong amplitude

Quantum dot expands →
Monopole oscillation
around new configuration
(Breathing mode)

New configuration, shape

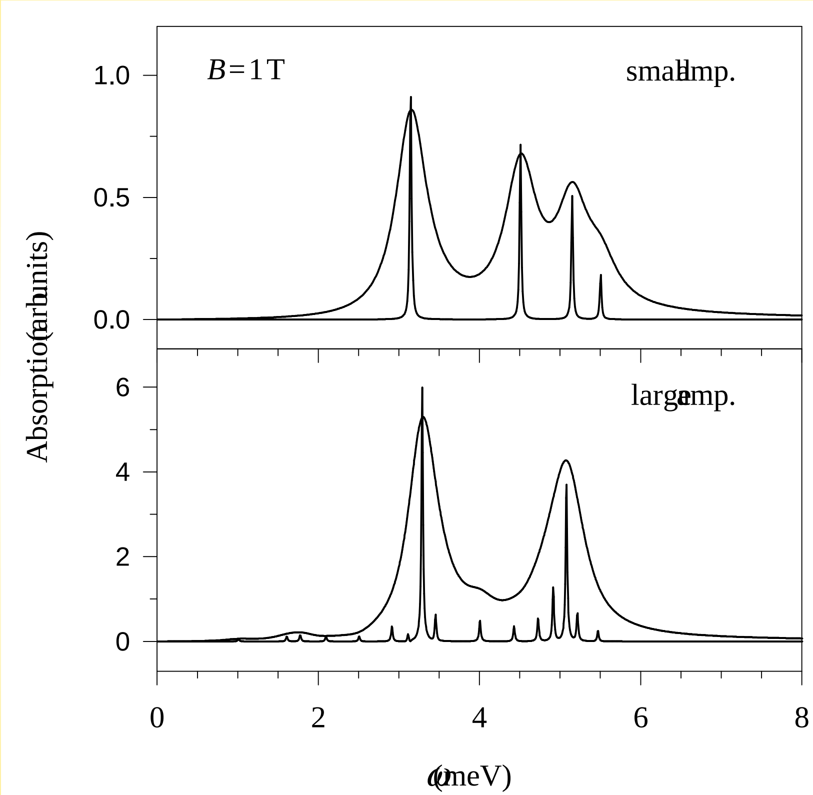
⇓

Modified dipole absorption

Large fluctuations of
mean field

⇓

Large variations in effective
single-particle energies



Two peak widths

Time window after expansion "Below-Kohn mode" vanishes

- In this approach no dissipation is included in the system, continuous input of energy as in a harmonic field would not describe all situations.
- Instead of a grid one could use a time-dependent basis.
- For a potential periodic in time one can consider Floquet's states, a convenient basis for time-harmonic systems. Self-consistent Floquet states for periodically driven quantum wells, B. Galdrikian, M. Sherwin, and B. Birnir, Phys. Rev. B 49, 13744-13749 (1994).
- For a "weak" time-dependent potential we can use linear response, R. Kubo, J. Phys. Soc. japan **12**, 570 (1957), Local Density-Functional Theory of Frequency-Dependent linear Response, E. K. U. Gross and Walter Kohn, Phys. Rev. Letters **55**, 2850 (1985).

Linear response

We know $\{ |\alpha\rangle, \epsilon_\alpha \}$ for the system described with

$$H_0|\alpha\rangle = \epsilon_\alpha|\alpha\rangle$$

$|\alpha\rangle$ are single-electron states, (no interaction or mean field description of an interacting system). We add a time-dependent potential

$$\delta V(t) = \delta E e^{-i(\omega+i\eta)t}, \qquad H(t) = H_0 + \delta V(t)$$

$\eta \to 0^+$, the external potential is switched on,

$$\lim_{t\to-\infty} H(t) = H_0.$$

H_0 contains a kinetic term, confinement, and effective MF potential.

In this effective single-electron picture we can use for the density operator (líkindavirkja)

$$\rho(t \to -\infty) = \rho_0 = f(H_0)$$

where f is the fermi distribution. The equation of motion for ρ is

$$i\hbar\dot{\rho}(t) = [H(t), \rho(t)] = [H_0, \rho(t)] + [\delta V(t), \rho(t)]$$

which becomes

$$i\hbar\delta\dot{\rho}_{\alpha,\beta}(t) = (\epsilon_\alpha - \epsilon_\beta)\delta\rho_{\alpha,\beta}(t) + \langle\alpha|[\delta V(t), \rho_0 + \delta\rho(t)]|\beta\rangle$$

an exact matrix version of the equation of motion for ρ

We linearize this equation in δV

$$i\hbar\delta\dot{\rho}_{\alpha,\beta}(t) = (\epsilon_\alpha - \epsilon_\beta)\delta\rho_{\alpha,\beta}(t) + (f_\beta - f_\alpha)\langle\alpha|\delta V(t)|\beta\rangle$$

with $f_\alpha = f(\alpha)$. We use a fourier transform

$$A(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega' e^{-i(\omega'+i\eta)t} A(\omega')$$

that transforms the equation into

$$\hbar(\omega' + i\eta)\delta\rho_{\alpha,\beta}(\omega') = \hbar(\omega_\alpha - \omega_\beta)\delta\rho_{\alpha,\beta}(\omega') + (f_\beta - f_\alpha)\langle\alpha|\delta V(\omega')|\beta\rangle$$

or

$$\hbar(\omega' + (\omega_\beta - \omega_\alpha) + i\eta)\delta\rho_{\alpha,\beta}(\omega') = (f_\beta - f_\alpha)\langle\alpha|\delta V(\omega')|\beta\rangle$$

Thus we have

$$\delta\rho_{\alpha,\beta}(\omega') = \frac{1}{\hbar}\left[\frac{(f_\beta - f_\alpha)}{\omega' + (\omega_\beta - \omega_\alpha) + i\eta}\right]\langle\alpha|\delta V(\omega')|\beta\rangle$$

We have also for the time-dependent potential, (the external potential)

$$\delta V(\omega') = \int_{-\infty}^{\infty} dt\, e^{i\omega' t}\delta V(t) \int_{-\infty}^{\infty} dt\, e^{i(\omega-\omega')t}\delta V = 2\pi\delta(\omega-\omega')\delta V$$

or simply

$$\langle\alpha|\delta V(\omega')|\beta\rangle = 2\pi\delta(\omega-\omega')\langle\alpha|\delta V|\beta\rangle$$

Fourier transform back to t

$$\delta\rho_{\alpha,\beta}(t) = \frac{1}{\hbar}\left[\frac{(f_\beta - f_\alpha)}{\omega + (\omega_\beta - \omega_\alpha) + i\eta}\right]\langle\alpha|\delta V|\beta\rangle e^{-i\omega t+\eta t} = \delta\rho_{\alpha,\beta}e^{-i\omega t+\eta t}$$

- The system responds at the same frequency as excited!
  Later we see that a finite system does not only respond at the same wavelength as excited.
- The system is thrown out of equilibrium by $\delta V(t)$.
  By $\delta\rho$ we have calculated a nonequilibrium change to the equilibrium fermi distribution!
- η is linked to power dissipation.
- How do we use this?

How does $\delta V(t)$ change $n(\mathbf{r})$?

In equilibrium, no $\delta V(t)$

$$n(\mathbf{r}) = \langle \delta(\hat{\mathbf{r}} - \mathbf{r}) \rangle = \mathrm{tr}(\delta(\hat{\mathbf{r}} - \mathbf{r})\rho_0) = \sum_\alpha \langle \alpha | \delta(\hat{\mathbf{r}} - \mathbf{r}) \rho_0 | \alpha \rangle$$

$$= \sum_{\alpha,\beta} \langle \alpha | \delta(\hat{\mathbf{r}} - \mathbf{r}) | \beta \rangle \langle \beta | \rho_0 | \alpha \rangle$$

$$= \sum_{\alpha,\beta} \int d\mathbf{r}' \langle \alpha | \mathbf{r}' \rangle \langle \mathbf{r}' | \delta(\hat{\mathbf{r}} - \mathbf{r}) | \beta \rangle \langle \beta | \rho_0 | \alpha \rangle$$

$$= \sum_{\alpha,\beta} \int d\mathbf{r}' \psi_\alpha^*(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}) \psi_\beta(\mathbf{r}') \rho^0_{\beta,\alpha} = \sum_\alpha f_\alpha |\psi_\alpha(\mathbf{r})|^2 = n(\mathbf{r})$$

Out of equilibrium, with $\delta V(t)$, then $n(\mathbf{r},t) = n(\mathbf{r}) + \delta n(\mathbf{r},t)$ with

$$\delta n(\mathbf{r},t) = \sum_{\alpha,\beta} \psi_\alpha^*(\mathbf{r})\psi_\beta(\mathbf{r})\delta\rho_{\beta,\alpha}(t)$$

or

$$\delta n(\mathbf{r},\omega) = \sum_{\alpha,\beta} \psi_\alpha^*(\mathbf{r})\psi_\beta(\mathbf{r})\frac{1}{\hbar}\left[\frac{(f_\alpha - f_\beta)}{\omega + (\omega_\alpha - \omega_\beta) + i\eta}\right]\langle\beta|\delta V|\alpha\rangle$$

$$= \sum_{\alpha,\beta}\int d\mathbf{r}'\psi_\alpha^*(\mathbf{r})\psi_\beta(\mathbf{r})\frac{1}{\hbar}\left[\frac{(f_\alpha - f_\beta)}{\omega + (\omega_\alpha - \omega_\beta) + i\eta}\right]\psi_\beta^*(\mathbf{r}')\delta V(\mathbf{r})\psi_\alpha(\mathbf{r}')$$

or

$$\delta n(\mathbf{r},\omega) = \int d\mathbf{r}'\chi(\mathbf{r},\mathbf{r}',\omega)\delta V(\mathbf{r}')$$

where $\chi(\mathbf{r},\mathbf{r}',\omega)$ is the retarded density response function of the system.

- So we have a formalism for calculating the nonequilibrium response of a system in the linear regime.
- External ...
  - Potential $\rightarrow$ density response $\rightarrow$ dielectric function.
  - Magnetic field $\rightarrow$ magnetization $\rightarrow$ susceptibility.
  - Vector potential $\rightarrow$ current response $\rightarrow$ conduction.
  - ...

But, in a MF description the change in f.ex. density $\delta n(\mathbf{r}, \omega)$ creates an internal induced potential $\rightarrow$ this has to be calculated self-consistently, next...