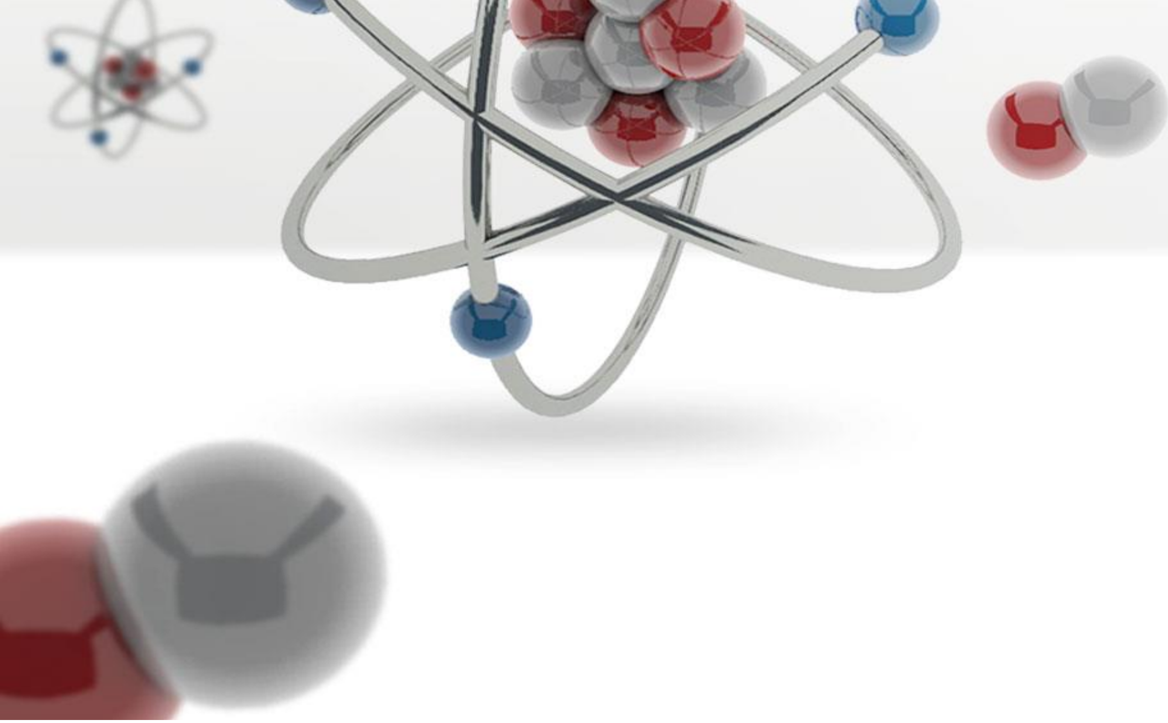

Computational Methods for Quantum Many-Body Systems (CMQMB) - from artificial atoms to high-temperature superconductors

Lecture 3 – Pictures of time evolution, linear response and Kubo formalism

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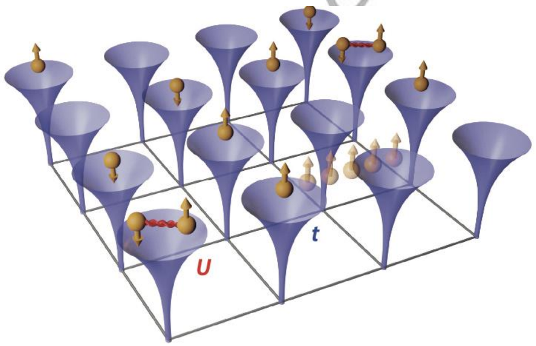
The full solid-state Hamiltonian



$$H/E_0 = \boxed{-\frac{1}{2}\sum_i \frac{\partial^2}{\partial \tilde{\boldsymbol{r}}_i^2}} - \frac{1}{2}\sum_k \frac{m}{M_k}\frac{\partial^2}{\partial \tilde{\boldsymbol{R}}_k^2} \boxed{+ \sum_{i<j} \frac{1}{|\tilde{\boldsymbol{r}}_i - \tilde{\boldsymbol{r}}_j|}} + \sum_{k<l} \frac{Z_k Z_l}{\left|\tilde{\boldsymbol{R}}_k - \tilde{\boldsymbol{R}}_l\right|} - \sum_{i,k} \frac{Z_k}{\left|\tilde{\boldsymbol{r}}_i - \tilde{\boldsymbol{R}}_k\right|}$$

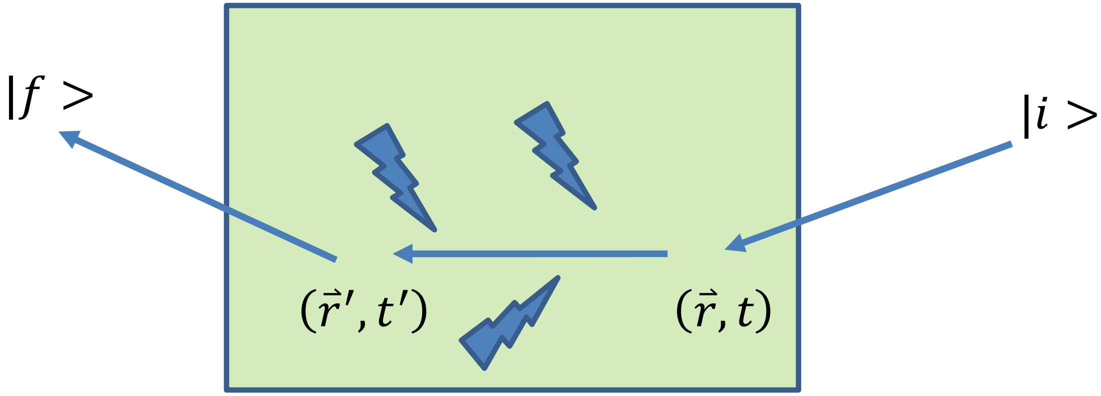
Many fascinating phenomena like magnetism, superconductivity, quantum criticality, metal-insulator transitions, …

However: advanced description necessary! One-particle picture does not hold!

Towards interacting systems…

How can we obtain information from an interacting system?

→ Scattering experiments (theory)



<u>Three ingredients necessary:</u>

1) Many-body treatment → Second quantization ✓
2) Time evolution → Pictures of time evolution
3) How does the system respond? → Linear response theory

Lecture 3

Content and goals

- Pictures of time evolution in quantum mechanics
  - Schrödinger picture
  - Heisenberg picture
  - Dirac picture
- Linear Response Theory
  - Kubo-Nakano formula
  - Examples

Lecture 3: Examples for correlation functions I

Density operator and variation of chemical potential

$$B(t) = -\int d^d r \, n(\vec{r})\delta\mu(\vec{r},t)$$

We also measure density: A=B

$$\delta\langle n(\vec{r})\rangle = \int_{-\infty}^{\infty} dt' \int d^d r' \chi_{nn}(\vec{r}-\vec{r}', t-t')\delta\mu(\vec{r}', t')$$

Density-density (or charge) response function
“Polarizability”

$$\chi_{nn}(\vec{r}-\vec{r}', t-t') = -i\theta(t-t')\langle[n(\vec{r},t), n(\vec{r}',t')]\rangle$$

Lecture 3: Examples for correlation functions II

Magnetic moment and external magnetic field in direction α

$$B(t) = -\int d^d r \;\, \mu_B g S_\alpha \cdot h_\alpha(\vec{r}', t')$$

We also measure spin: A=B

Spin-spin (or magnetic) response function
“spin susceptibility”

$$\chi_{S_\alpha S_\beta}(\vec{r} - \vec{r}', t - t') = -i\theta(t - t')\left\langle \left[S_\alpha(\vec{r}, t), S_\beta(\vec{r}', t') \right] \right\rangle$$