(R. M. Chapter 6)

Now detour to alternative representation

Correlation functions $\longleftrightarrow$ wave function

Some basic properties of the many body W.F.

Most of physical observables can be described by correlation functions.
However W.F. carries much more information and is very useful in proving many basic theorems.
If we know the W.F. we can calculate any correlation function.

(Succesfull examples: • Laughlin W.F. for fractional quantum Hall effect
• BCS W.F. for superconductors)

If we know all two particle (and single particle) correlation functions we still can not write down the wave function

How hard is to tabulate the W.F. for N electrons?
$3N$ dimensional function. Assume each dimension requires 100 basis functions
then $(100)^{3N}$ complex numbers.

Lets write $\Phi(\vec{r}_1 z_1, \vec{r}_2 z_2, \vec{r}_3 z_3, \cdots \vec{r}_N z_N) = \Phi(x_1, x_2, \cdots x_N) \equiv \Phi(X)$

Here we will use $(\vec{r}_i, z_i) \equiv x_i$ and $X = \{x_1, x_2, \cdots x_N\}$

Below we will list basic properties of the multiparticle wave function.

Properties of multiparticle Φ for fermions

1) Antisymmetry: $\Phi(x_2, x_1, \dots) = -\Phi(x_1, x_2, \dots)$

2) Obeys symmetry of the associate space group

- normally group of H, if no broken symmetry.

Operator A: If $[H, A] = 0$ then

$H\Phi = E\Phi$

and $A\Phi = a\Phi$ simultaneously eigenfunction of both, a is a good quantum number

3) Continuity: Wave function and all of their derivatives $\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \dots\right)$ are continuous at all points, except at points of coincidence. These are points where $\vec{r}_i = \vec{r}_j$ (for two electrons) or $\vec{r}_i = \vec{R}_j$ (electron at a nucleus).

4) At points of coincidence, the wave function satisfies the "Cusp condition" (Non-analytic points in space, which cause very slow convergence of most basis sets)

We can fix all points $\vec{r}_3, \vec{r}_4, \dots \vec{r}_N$ except $\vec{r}_1$ and $\vec{r}_2$. We express the relevant part of the Hamiltonian in terms of in terms of $\vec{r}_1, \vec{r}_2$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$

After long calculation, one can obtain:

$$(\vec{\nabla}_1^2 + \vec{\nabla}_2^2) = \left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + \right.$$

$$+ 2\,\hat{r}_1 \cdot \hat{r}_{12}\frac{\partial^2}{\partial r_1 \partial r_{12}} + 2\,\hat{r}_2 \cdot \hat{r}_{12}\frac{\partial^2}{\partial r_2 \partial r_{12}} +$$

$$\left. + \frac{4}{r_{12}}\frac{\partial}{\partial r_{12}} + 2\frac{\partial^2}{\partial r_{12}^2}\right)$$

(usual ∇^2 in spherical coordinates)

= diverges when $r_1 \to 0$

= diverges when $r_{12} \to 0$

$$H = -\tfrac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{e^2}{r_{12}} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \dots$$

$$H = \dots\dots - \tfrac{1}{2}\frac{2}{r_1}\frac{\partial}{\partial r_1} - \frac{Ze^2}{r_1} - \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} + \frac{e^2}{r_{12}} + \dots$$

We must have $H\Phi \leq \infty$ therefore

$$\frac{1}{r_1}\left(\frac{\partial}{\partial r_1} + Ze^2\right)\Phi = \text{const}$$

$$\frac{1}{r_{12}}\left(\frac{\partial}{\partial r_{12}} - \frac{e^2}{2}\right)\Phi = \text{const}$$

Cusp condition is e) $\frac{\partial \phi}{\partial r_1} = -Ze^2 \phi \Big|_{r_1 = R_1} \Rightarrow \phi(\vec{r}_1, \vec{r}_2, \ldots) \approx e^{-Ze^2|\vec{r}_1 - \vec{R}_1|} \phi(\vec{R}_1, \vec{r}_2, \ldots)$

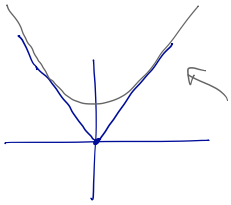
we set $R_1 = 0$ above

b) $\frac{\partial \phi}{\partial r_{12}} = \frac{e^2}{2} \phi \Big|_{r_1 = r_2} \Rightarrow \phi(\vec{r}_1, \vec{r}_2, \ldots) \approx \frac{e^2}{2} |\vec{r}_1 - \vec{r}_2| \, \phi(\vec{r}_1, \vec{r}_1, \ldots)$

check $\phi|_{r_1 = r_2} \approx \frac{e^2}{2} r_{12} \phi^0$

$\frac{\partial \phi}{\partial r_{12}} \approx \frac{e^2}{2} \phi^0$

cusp, non-analytic



very hard to approximate with any finite basis set.

Also the two particle response function are affected by cusp

$\chi(\vec{r}_1, \vec{r}_2) \equiv \chi(\vec{r}_1 - \vec{r}_2)$ in homogeneous system

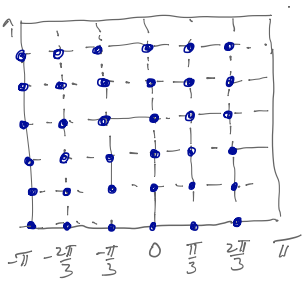
$\chi(\vec{r}_1 - \vec{r}_2)$ non-analytic in r_{12}.

$\chi(q) \sim \frac{1}{q^2} \Rightarrow \chi(r_{12}) \sim \frac{1}{r_{12}}$ very slow fall-off

5) If no SOC and no B field
then ϕ can be chosen real.
Otherwise ϕ is complex.
However, complex ϕ might have better convergence properties.
So called "twisted boundary condition" can make finite system a better approximation for infinite system. It is also crucial if the system has finite polarization ("Modern theory of polarization" is based on the Berry phase)

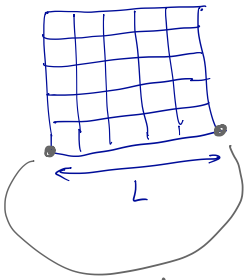
Example: uniform electron gas with spherical fermi surface and 6×6 sites in 2D. The first BZ would look like:

periodic boundary conditions



36 k-points

$$\vec{k} = \left(\frac{n_1}{N_1} 2\pi, \frac{n_2}{N_2} 2\pi\right)$$



real space

differ for phase e^{ikL}

periodic boundary condition

$$\phi(\vec{r}_1 + L\vec{e}_x, \vec{r}_2, \dots) = \phi(\vec{r}_1, \vec{r}_2, \dots)$$

twisted boundary condition

$$\phi_{\vec{k}}(\vec{r}_1 + L\vec{e}_x, \vec{r}_2 \dots) = e^{i(k_x L)} \phi(\vec{r}_1, r_2, \dots)$$

$k_x L = \vartheta_x$

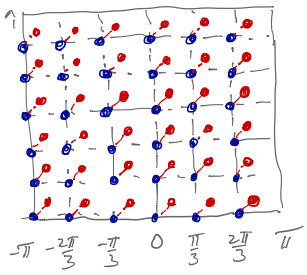
where $\vartheta \in [-\pi, \pi]$ freedom

Condition for periodicity

$$L \cdot n_1 = 2M\pi + \vartheta$$

$$L = a \cdot N$$

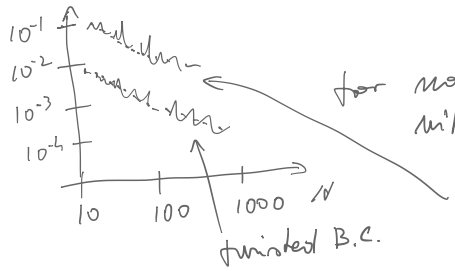
$$n_1 a = \frac{2M\pi + \vartheta}{N}$$



shifted mesh for $\vartheta_x = \frac{\pi}{2}$ and $\vartheta_y = \frac{\pi}{2}$

Used in electronic structure calculations for better convergence.

E - Exact



for non-interacting system with 13 electrons

not twisted B.C.

There is a more important property associated with the twisted phase. It can distinguish metals from insulators.

Kohn proposed: a) In insulators the energy is independent of the twist (because electrons are localized)

We can define the "center of mass" $\langle R_{cm} \rangle$ which is well defined, and gives polarization of the system.

$$\langle R_{cm}^2 \rangle - \langle R_{cm} \rangle^2 < \infty$$

b) In metals the energy increases with the twist

$E + = 2D V^{1/3} \vartheta^2$ where D is the Drude weight.

and $\langle R_{cm} \rangle$ is not well defined so that

$\langle R_{cm}^2 \rangle - \langle R_{cm} \rangle^2 = \infty$ and the system has net velocity.

The center of mass is proportional to polarization of the system, and is given by the Berry phase. It was first derived by David Vanderbilt in his "modern theory of polarization."

$$\langle \Delta R_{cm}^{\alpha} \rangle = \frac{2 V_{cell}}{(2\pi)^3} \int d^3 k \, \mathrm{Im} \left\{ \langle u_k^f | \partial_{k_\alpha} | u_k^f \rangle - \langle u_k^i | \partial_{k_\alpha} u_k^i \rangle \right\}$$

$\alpha = x, y, z$

final, initial

Here $u_k(\vec{r}_1, \vec{r}_2, \ldots) = e^{-i \sum_j \vec{k} \vec{r}_j} \phi(\vec{r}_1, \vec{r}_2, \ldots)$

phase factor; ϕ: eigenstate of H

with $u_k(\vec{r}_1, \vec{r}_2, \ldots)$ periodic in V_{cell}.

in complete analogy with non-interacting system, where $\psi_k(\vec{r}) = e^{-i \vec{k} \vec{r}} u_k(\vec{r})$ with $u(\vec{r})$ periodic in V_{cell}

$$\langle (\Delta R_{cm}^{\alpha})^2 \rangle = \frac{V_{cell}}{(2\pi)^3} \int d^3 k \, \mathrm{Re} \left\{ \langle \partial_{k_\alpha} u_k | \partial_{k_\alpha} u_k \rangle - \langle u_k | \partial_{k_\alpha} u_k \rangle \langle \partial_{k_\alpha} u_k | u_k \rangle \right\}$$