Broken-symmetry insulators: General theory and collective modes

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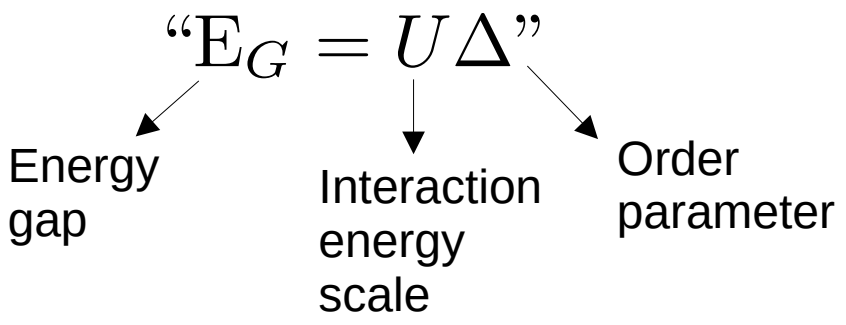
MagLab Winter school 2023

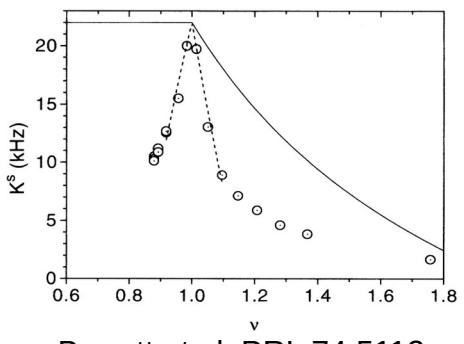
Broken-symmetry insulator = An electronic system with a gap to all charged excitations which is a direct consequence of spontaneous symmetry breaking.



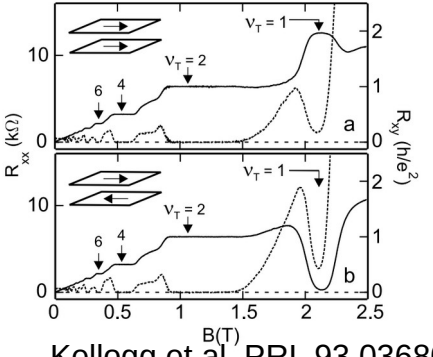
Often these states break exact or approximate continuous symmetries (e.g U(1) or SU(2)), so they have Goldstone modes (e.g. spin waves) or other low-energy collective modes.

Examples of broken-symmetry insulators:

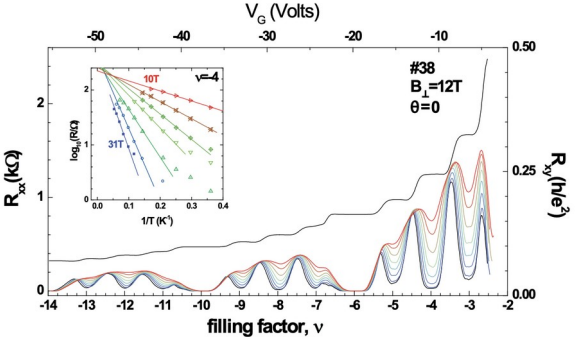
- Quantum Hall ferromagnets and exciton superfluids
  [both in 2DEGs in semi-conductor structures and in graphene]



Barrett et al. PRL 74 5112



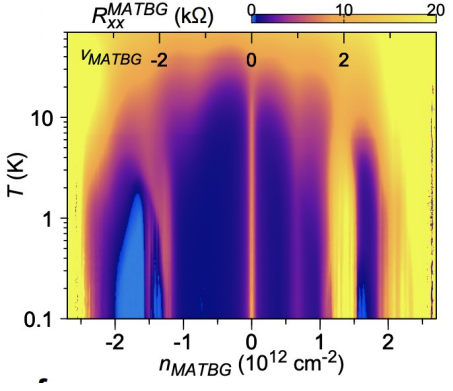
Kellogg et al. PRL 93 036801

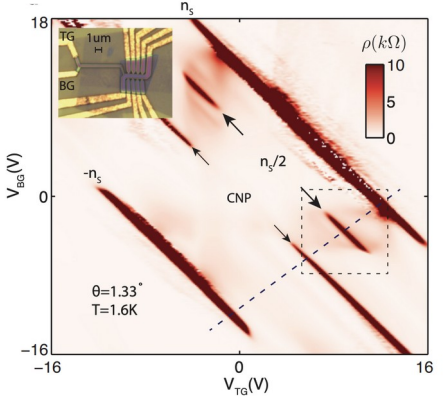


Young et al. Nature Physics 8, 550

- Insulating states in moire flat bands [both in graphene and TMD materials]

Park et al.
Nature 592





Liu et al.
Nature 583

Outline:

- Mean-field (Hartree-Fock) theory of broken-symmetry insulators
- The Hartree-Fock path integral and fluctuations beyond mean-field
- Collective modes

Mean-field (Hartree-Fock) theory of broken-symmetry insulators

Hartree-Fock = Variational energy minimization with Slater determinants

Slater determinant: $|\psi\rangle = \prod_{a=1}^{N} c_a^\dagger |0\rangle$

$$c_i^\dagger = \sum_{a=1}^{N} M_{ia} c_a^\dagger \Rightarrow \prod_{i=1}^{N} c_i^\dagger |0\rangle = \det(M) \prod_{a=1}^{N} c_a^\dagger |0\rangle$$

A Slater determinant is in one-to-one correspondence with a single-particle correlation matrix:

$$P_{ab} := \langle c_b^\dagger c_a \rangle \,, \; P^2 = P$$

$$H = \sum_{a,b} T_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{a,b,c,d} V_{ab,cd} c_a^\dagger c_c^\dagger c_d c_b \quad \text{with} \quad \begin{cases} V_{ab,cd} = V_{ba,dc}^* \\ V_{ab,cd} = V_{cd,ab} \end{cases}$$

Using Wick's theorem, the energy of a Slater determinant with SP correlation matrix P is found to be:

$$E[P] = \mathrm{tr}(TP) + \frac{1}{2} \sum_{a,b,c,d} (V_{ab,cd} - V_{ad,cb}) P_{ba} P_{dc}$$

Hartree-Fock is a constrained optimization problem: minimize E[P] subject to the constraint that $P^2 = P$. So we have to extremize the following cost function:

$$C[P] = E[P] + \mathrm{tr}(X(P^2 - P))$$

Lagrange multipliers

$$\frac{\partial C}{\partial P} = 0 \Rightarrow H_{HF}[P] + XP + PX - X = 0 \Rightarrow [H_{HF}[P], P] = 0$$

$$H_{HF}[P]_{ab} = T_{ab} + \sum_{c,d} (V_{ab,cd} - V_{ad,cb}) P_{dc} \longrightarrow \text{Mean-field Hamiltonian}$$

$$H_{HF}[P]_{ab} = T_{ab} + \sum_{c,d}(V_{ab,cd} - V_{ad,cb})P_{dc}$$

$$[H_{HF}[P], P] = 0$$

Hartree-Fock self-consistency equation:

The interaction is replaced with a mean-field. The same electrons that move through the mean-field should also generate the mean-field.

Another physical interpretation of the self-consistency equation is provided by

Brillouin's theorem: If $|\psi\rangle$ is a Slater determinant satisfying the HF self-consistency equation, then $H|\psi\rangle$ is orthogonal to all states with a single particle-hole excitation.

Work in the basis where P is diagonal: $P_{\alpha\beta} = P_\alpha \delta_{\alpha\beta}\ ,\ H_{HF}[P]_{\alpha\beta} = \delta_{\alpha\beta}E_\alpha$

$i, j, k, l, \ldots \longrightarrow$ Occupied states $(P_i = 1)$

$m, n, o, p, \ldots \longrightarrow$ Unoccupied states $(P_m = 0)$

State with a single PH excitation: $c_m^\dagger c_i |\psi\rangle$

$$\Rightarrow \langle\psi|c_i^\dagger c_m H|\psi\rangle = (1 - P_m)H_{HF}[P]_{mi}P_i = 0$$

The energy of the self-consistent Hartree-Fock state is given by

$$E[P] = \frac{1}{2}\mathrm{tr}\left(P(T + H_{HF}[P])\right)$$

and NOT by the sum of the occupied single-particle energies of the mean-field Hamiltonian.

The energies of the mean-field Hamiltonian do have a physical meaning, due to

Koopmans' theorem: The energies of the mean-field Hamiltonian correspond to the mean-field energies for removing or adding a single electron to the system.

Hartree-Fock ground state energy: $E_0^N = \sum_i T_{ii} + \frac{1}{2}\sum_{i,j}(V_{ii,ij} - V_{ij,ji})$

Energy with electron in state k removed: $E_k^{N-1} = \sum_{i\neq k} T_{ii} + \frac{1}{2}\sum_{i,j\neq k}(V_{ii,ij} - V_{ij,ji})$

$$E_k^{N-1} - E_0^N = -T_{kk} - \sum_i (V_{ii,kk} - V_{ik,ki}) = -E_k$$

Optimal Damping Algorithm (ODA)

Canonical Hartree-Fock problem: min E[P], subject to $P^2 = P$ and tr(P) = N

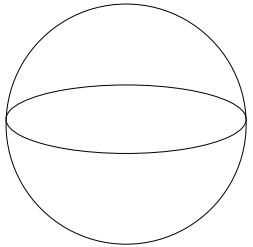
ODA is a simple numerical algorithm which is guaranteed to converge to a solution of this optimization problem. The key insight is to relax the constraints to $P^2 \leq P$ and tr(P) = N. The matrices P which satisfy these constraints form a convex set **S**, the convex hull of which are projectors.

S is a convex set if for $P, Q \in \mathbf{S} \Rightarrow \lambda P + (1-\lambda)Q \in \mathbf{S} \text{ for } \lambda \in [0,1]$

Example: One electron in a two-dimensional Hilbert space consisting of two orbitals.

A general SP correlation matrix can be written as $P = U^\dagger \sigma^z U \ , \ U \in \mathrm{SU}(2)$

The space of projectors is thus given by SU(2)/U(1) = S^2



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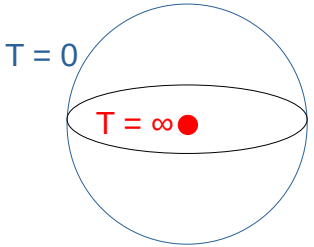

The convex set of 2x2 matrices P with trace one and which satisfy $P^2 = P$ is then simply the ball with boundary S^2

Optimal Damping Algorithm (ODA)

1) Take a matrix P_1 from **S**
2) Construct the Hartree-Fock mean-field Hamiltonian from P_1
3) Diagonalize the mean-field Hamiltonian, and denote the SP correlation matrix obtained from filling the N lowest energy states as P_2
4) Define $P(\lambda) = (1-\lambda)P_1 + \lambda P_2$
5) Minimize $E(\lambda) = E[P(\lambda)] = E[P_1] + C_1 \lambda + C_2 \lambda^2/2$ over the interval [0,1]. Denote the optimal λ as λ_{min} .
6) if $E[P_1] - E(\lambda_{min}) < \epsilon$:
   STOP
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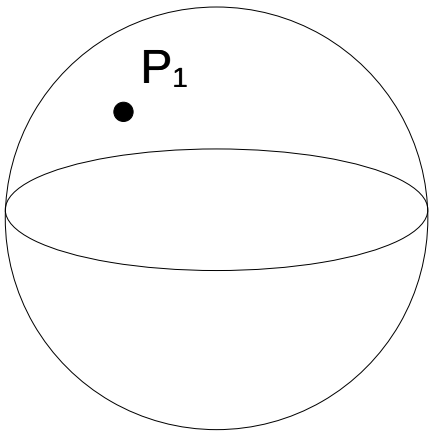

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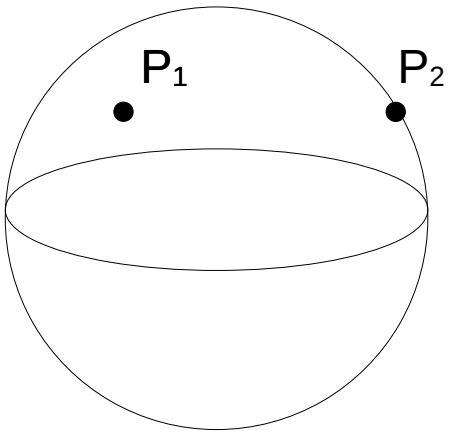

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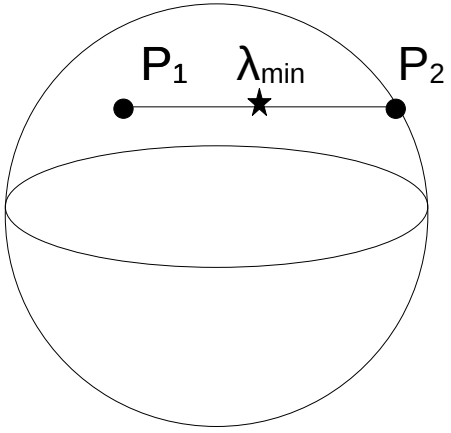

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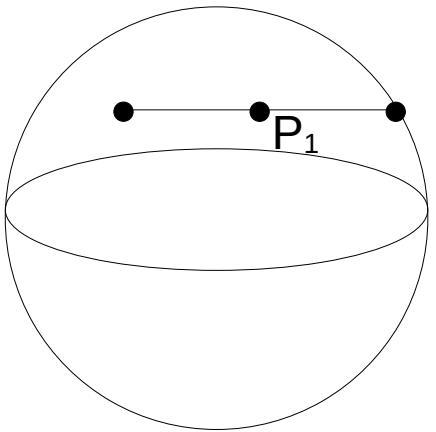

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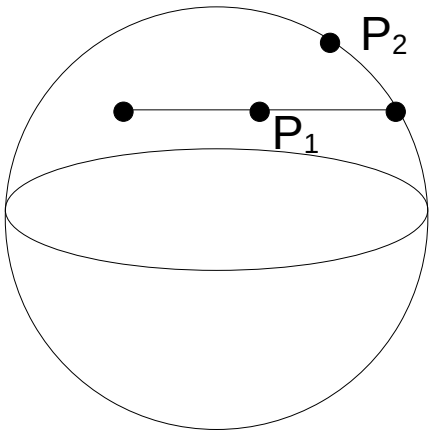

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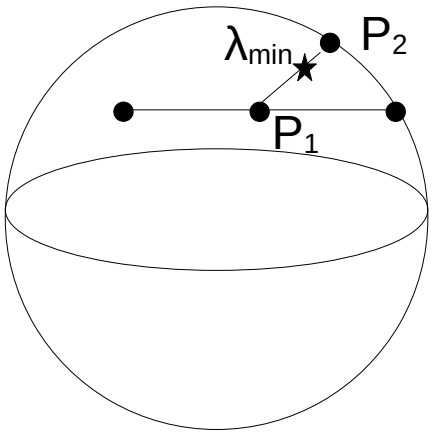

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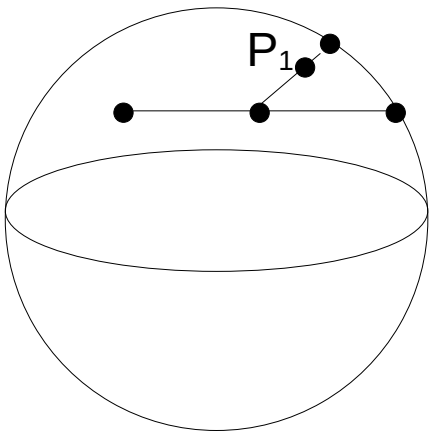


Optimal Damping Algorithm (ODA)

The ODA algorithm is guaranteed to converge (this statement requires a proof which is not given here). Furthermore, by construction, the energy decreases during every iteration.

Due to the nature of the algorithm, it is clear that the final converged state lies on the convex hull, and is therefore a valid SP correlation matrix corresponding to a particular Slater determinant.

For further details: J. Chem. Phys. 116, 8255

Stability of a self-consistent Hartree-Fock state

Thouless' theorem: Every Slater determinant which is not orthogonal to a given Slater determinant $|\psi_0\rangle$ can be written as

$$|\psi(M)\rangle \propto \exp\left(\sum_{m,i} M_{mi} c_m^\dagger c_i\right) |\psi_0\rangle$$

Moreover, the matrix M is unique.

Proof: Consider a Slater determinant which consists of N occupied states labeled by a. It can be written as

$$|\psi\rangle = \prod_{a=1}^{N} \left(\sum_{i=1}^{N} f_{ai} c_i^\dagger + \sum_m f_{am} c_m^\dagger\right) |0\rangle$$

As this state is assumed not to be orthogonal to the reference state, we have

$$\langle\psi|\psi_0\rangle = \det(f_{ai}) \neq 0$$

Stability of a self-consistent Hartree-Fock state

Denote the inverse of the NxN matrix f_{ai} as F, and define $M_{mi} = \sum_{a=1}^{N} F_{ia} f_{am}$

We can now write

$$
\begin{aligned}
|\psi\rangle &= \prod_{a=1}^{N} \left(\sum_{i=1}^{N} f_{ai} c_i^\dagger + \sum_{m} f_{am} c_m^\dagger \right) |0\rangle \\
&= \det(f_{ai}) \prod_{i=1}^{N} \left(c_i^\dagger + \sum_{m} M_{mi} c_m^\dagger \right) |0\rangle \\
&\propto \prod_{i=1}^{N} \left(1 + \sum_{m} M_{mi} c_m^\dagger c_i \right) c_i^\dagger |0\rangle \\
&= \prod_{i=1}^{N} \prod_{m} \left(1 + M_{mi} c_m^\dagger c_i \right) c_i^\dagger |0\rangle \\
&= e^{\sum_{m,i} M_{mi} c_m^\dagger c_i} |\psi_0\rangle
\end{aligned}
$$

Stability of a self-consistent Hartree-Fock state

If our reference state is a local minimum in the Hartree-Fock variational energy landscape, then it should follow that

$$\frac{\langle\psi(M)|H|\psi(M)\rangle}{\langle\psi(M)|\psi(M)\rangle} - \langle\psi_0|H|\psi_0\rangle \geq 0$$

for small M.

One finds:

$$\langle\psi(M)|\psi(M)\rangle = 1 + \sum_{m,i} |M_{mi}|^2 + \mathcal{O}(M^4)$$

$$\langle\psi(M)|H|\psi(M)\rangle = \langle\psi_0|H|\psi_0\rangle \left(1 + \sum_{m,i} |M_{mi}|^2\right) + \frac{1}{2}(M^*, M) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} M \\ M^* \end{pmatrix} + \mathcal{O}(M^3)$$

The linear term vanishes for solutions to the self-consistency equation due to Brillouin's theorem.

Stability of a self-consistent Hartree-Fock state

$$\langle\psi(M)|H|\psi(M)\rangle = \langle\psi_0|H|\psi_0\rangle \left(1 + \sum_{m,i} |M_{mi}|^2\right) + \frac{1}{2}(M^*, M) \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} M \\ M^* \end{pmatrix} + \mathcal{O}(M^3)$$

$$A_{im,jn} = (E_m - E_i)\delta_{ij}\delta_{mn} + V_{im,nj} - V_{ij,nm}$$

$$B_{im,jn} = V_{mi,nj} - V_{mj,ni}$$

Hermiticity of the Hamiltonian and the fermion anti-commutation relations imply that A is Hermitian, and B is symmetric.

The requirement that the self-consistent HF state is a local energy minimum is thus equivalent to

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \geq 0$$

This condition will play an important later in our discussion of collective modes.

The Hartree-Fock path integral and fluctuations beyond mean-field

Assume we have found a solution of the Hartree-Fock self-consistency equation corresponding to the following Slater determinant:

$$|\psi_0\rangle = \prod_i c_i^\dagger |0\rangle$$

Let us also rewrite the Hamiltonian in the basis of HF orbitals:

$$H = \sum_{\alpha,\beta} T_{\alpha\beta} c_\alpha^\dagger c_\beta + \frac{1}{2} \sum_{\alpha,\beta,\lambda,\sigma} V_{\alpha\beta,\lambda\sigma} c_\alpha^\dagger c_\lambda^\dagger c_\sigma c_\beta$$

We will now construct a Grassmann path integral representation of the partition function, but using the following unconventional coherent states:

$$|\bar{\psi}, \psi\rangle = \bigotimes_i |\bar{\psi}_i\rangle \bigotimes_m |\psi_m\rangle$$

$$|\psi_m\rangle = (1 - \psi_m c_m^\dagger)|0\rangle$$

$$|\bar{\psi}_i\rangle = (1 - \bar{\psi}_i c_i) c_i^\dagger |0\rangle$$

Conventional coherent states: $|\psi_m\rangle = (1 - \psi_m c_m^\dagger)|0\rangle$

$$
\begin{aligned}
c_n|\psi_n\rangle &= \psi_n|\psi_n\rangle \\
\langle\bar{\psi}_n|\psi_n\rangle &= \langle 0|(1 - c_n\bar{\psi}_n)(1 - \psi_n c_n^\dagger)|0\rangle = 1 + \bar{\psi}_n\psi_n = e^{\bar{\psi}_n\psi_n} \\
\int \mathrm{d}\bar{\psi}_n \mathrm{d}\psi_n \, e^{-\bar{\psi}_n\psi_n}|\psi_n\rangle\langle\bar{\psi}_n| &= \mathbb{1}
\end{aligned}
$$

Particle-hole transformed coherent states: $|\bar{\psi}_i\rangle = (1 - \bar{\psi}_i c_i)c_i^\dagger|0\rangle$

$$
\begin{aligned}
c_i^\dagger|\bar{\psi}_i\rangle &= \bar{\psi}_i|\bar{\psi}_i\rangle \\
\langle\psi_i|\bar{\psi}_i\rangle &= \langle 0|c_i(1 - c_i^\dagger\psi_i)(1 - \bar{\psi}_i c_i)c_i^\dagger|0\rangle = 1 + \psi_i\bar{\psi}_i = e^{\psi_i\bar{\psi}_i} \\
\int \mathrm{d}\psi_i\bar{\psi}_i e^{-\psi_i\bar{\psi}_i}|\bar{\psi}_i\rangle\langle\psi_i| &= \mathbb{1}
\end{aligned}
$$

Inserting resolutions of the identity as in the standard textbook construction of the Grassmann path integral we find:

$$Z(\beta) = \mathrm{tr}\left(e^{-\beta H}\right) = e^{-\beta E_0^{HF}} \int D\bar{\psi} D\psi \, e^{-S[\bar{\psi},\psi]}$$

$E_0^{HF} = \langle \psi_0 | H | \psi_0 \rangle$ Hartree-Fock energy

$$S = \int_0^\beta \mathrm{d}\tau \sum_\alpha \bar{\psi}_\alpha (\partial_\tau + E_\alpha)\psi_\alpha + \frac{1}{2} \sum_{\alpha\beta\lambda\sigma} V_{\alpha\beta\lambda\sigma} \bar{\psi}_\alpha \bar{\psi}_\lambda \psi_\sigma \psi_\beta$$

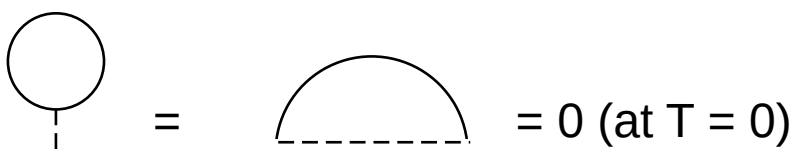
Mean-field single-particle energies

$$S = \int_0^\beta \mathrm{d}\tau \sum_\alpha \bar{\psi}_\alpha(\partial_\tau + E_\alpha)\psi_\alpha + \frac{1}{2}\sum_{\alpha\beta\lambda\sigma} V_{\alpha\beta\lambda\sigma}\bar{\psi}_\alpha\bar{\psi}_\lambda\psi_\sigma\psi_\beta$$

This action can now be used for standard perturbative diagrammatic calculations. At zeroth order, this will produce the mean-field result. For example, the free energy is given by

$$F = E_0^{HF} - T\sum_i \ln\left(1 + e^{\beta E_i}\right) - T\sum_n \ln\left(1 + e^{-\beta E_n}\right) + \mathcal{O}(V)$$

Note that due to the normal ordering with respect to the HF state, the Hartree and Fock self-energy diagrams are zero:



This ensures that we do not double-count the Hartree-Fock renormalization of the single-particle energies.

When is the HF path integral a useful starting point?

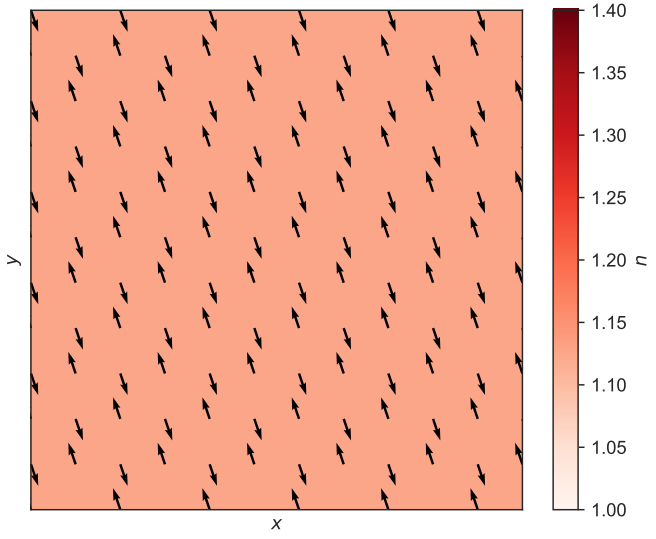
Example: Square lattice Hubbard model with next-nearest neighbour hopping:

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + h.c. - t' \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger c_j + h.c. + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

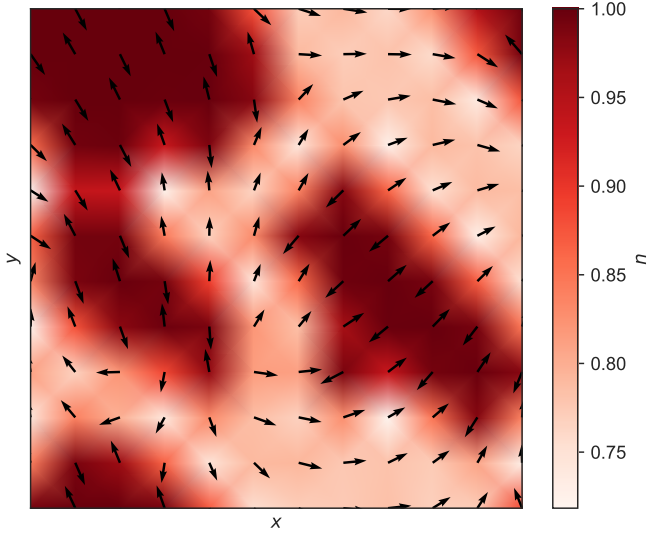
with $t'/t = -0.35\,,\ U/t = 10$

SCHF results at two different dopings:

$n = 1 + 1/8$

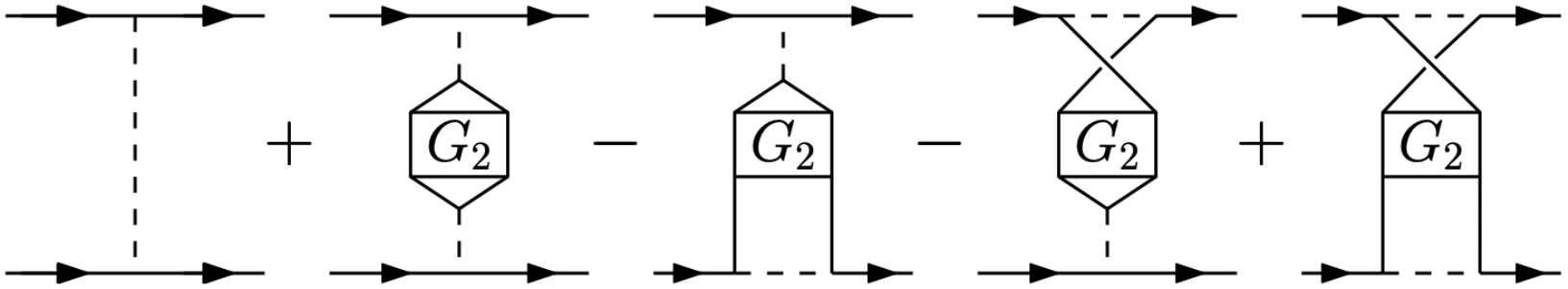


$n = 1 - 1/8$

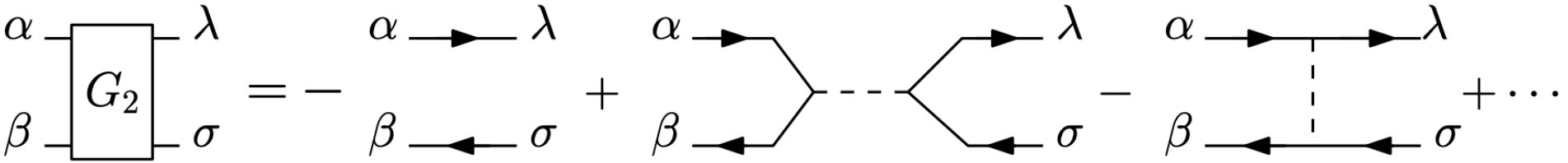


Collective modes

The effective RPA interaction that appears in diagrammatic calculations with the HF path integral is:

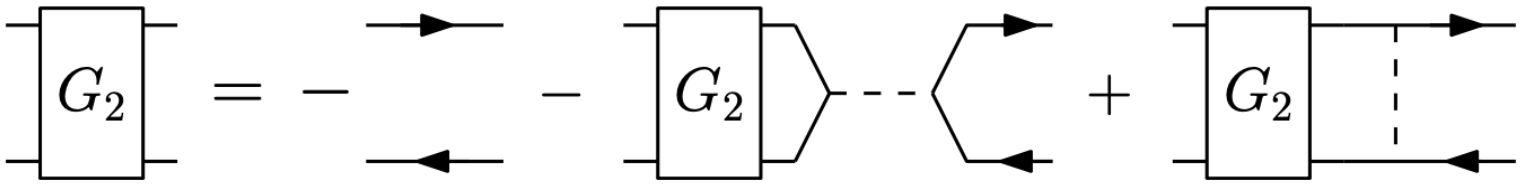


where G_2 is the following sum of RPA diagrams:



This sum includes many familiar diagrams such as bubble diagrams and Berk-Schrieffer diagrams.

Summing the infinite set of diagrams to obtain G_2 is equivalent to solving the following Bethe-Salpeter equation:



Written out explicitly, we find

$$
\begin{aligned}
G_2(\alpha,\beta;\lambda,\sigma;i\nu) &= T\sum_{\omega_n}\left(-\delta_{\beta\sigma}\delta_{\lambda\alpha}\frac{1}{i(\omega_n-\nu)-E_\beta}\frac{1}{i\omega_n-E_\alpha}\right) \\
&\quad +\sum_{\mu\nu}V_{\alpha\mu,\beta\nu}G_2(\nu,\mu;\lambda,\sigma;i\nu)T\sum_{\omega_n}\frac{1}{i(\omega_n-\nu)-E_\beta}\frac{1}{i\omega_n-E_\alpha} \\
&\quad -\sum_{\mu\nu}V_{\alpha\mu,\nu\beta}G_2(\nu,\mu;\lambda,\sigma;i\nu)T\sum_{\omega_n}\frac{1}{i(\omega_n-\nu)-E_\beta}\frac{1}{i\omega_n-E_\alpha} \\
&= -\frac{f(E_\beta)-f(E_\alpha)}{i\nu-E_\alpha+E_\beta}\left(\delta_{\alpha\lambda}\delta_{\beta\sigma}-\sum_{\mu\nu}\left(V_{\alpha\mu,\beta\nu}-V_{\alpha\mu,\nu\beta}\right)G_2(\nu,\mu;\lambda,\sigma;i\nu)\right)
\end{aligned}
$$

Fermi-Dirac distribution

At zero temperature, the Bethe-Salpeter equation becomes:

$$\sum_{\mu,\nu} \left((n_\beta - n_\alpha)(E_\alpha - E_\beta - i\nu)\delta_{\alpha\nu}\delta_{\beta\mu} + V_{\alpha\mu,\beta\nu} - V_{\alpha\mu,\nu\beta}\right) G_2(\nu,\mu;\lambda,\sigma;i\nu) = \delta_{\alpha\lambda}\delta_{\beta\sigma}$$

$n_\beta - n_\alpha$ → FD distribution at T=0, i.e. the occupation numbers

This equation can be rewritten as following matrix equation:

$$\begin{pmatrix} A - i\nu\mathbb{1} & B \\ B^* & A^* + i\nu\mathbb{1} \end{pmatrix} \begin{pmatrix} G^{(1)}(i\nu) & G^{(2)}(i\nu) \\ G^{(3)}(i\nu) & G^{(4)}(i\nu) \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}$$

with

$$\begin{aligned} G^{(1)}_{mi,nj}(i\nu) &= G_2(m,i;n,j;i\nu) \\ G^{(2)}_{mi,nj}(i\nu) &= G_2(m,i;j,n;i\nu) \\ G^{(3)}_{mi,nj}(i\nu) &= G_2(i,m;n,j;i\nu) \\ G^{(4)}_{mi,nj}(i\nu) &= G_2(i,m;j,n;i\nu) \end{aligned}$$

The matrices A and B are the same as we introduced previously in our discussion of the stability of a Hartree-Fock solution.

Writing $H_B = \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}$ the solution to the Bethe-Salpeter equation becomes

$$G_2(i\nu) = (ZH_B - i\nu\mathbb{1})^{-1} Z \text{ with } Z = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$$

To further simplify the solution, let us diagonalize ZH_B. We have that

$$ZH_B|\lambda\rangle = \lambda|\lambda\rangle \Rightarrow \langle\lambda|H_B|\lambda\rangle = \lambda\langle\lambda|Z|\lambda\rangle$$

From this equation it follows that the eigenvalues of ZH_B are real, except when $|\lambda\rangle$ is a null vector of H_B. From the positivity of H_B it also follows that the sign of λ is the same as the sign of $\langle\lambda|Z|\lambda\rangle$. These properties can be translated into the following matrix equations:

$$ZH_B = S(\hat{Z}\Omega)S^{-1} \text{ with } \hat{Z}_{\lambda,\lambda'} = \pm\delta_{\lambda,\lambda'}, \Omega_{\lambda,\lambda'} = \delta_{\lambda,\lambda'}\Omega_\lambda \geq 0$$

$$S^\dagger = \hat{Z}S^{-1}Z$$

The collective mode matrix H_B has the following particle-hole symmetry:

$$H_B^* = X H_B X \quad \text{with } X = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

this implies that the eigenvalues of ZH_B come in pairs with opposite signs $\hat{Z}_\lambda$, from which it follows that the Ω's come in degenerate pairs, with the corresponding eigenvectors related by particle-hole symmetry.

We can now write $G_2(i\nu) = (ZH_B - i\nu\mathbb{1})^{-1} Z$

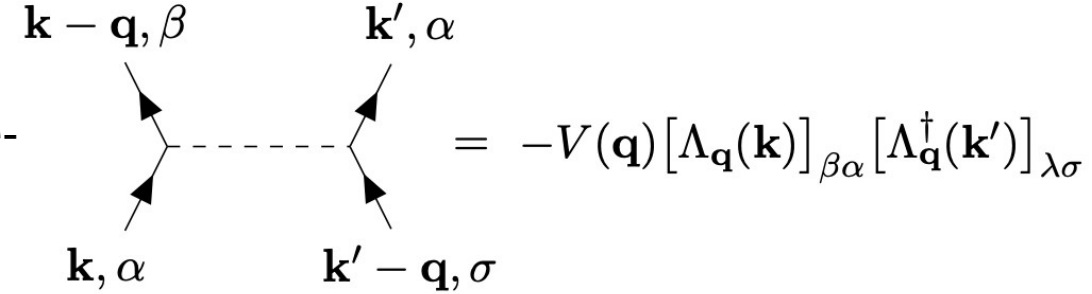
$$= S(\Omega - i\nu\hat{Z})\hat{Z}S^{-1}Z$$

$$= S(\Omega - i\nu\hat{Z})S^\dagger$$

This expression can be recognized as the propagator of the bosonic collective modes with energies Ω. The columns of S are the corresponding wavefunctions of the collective modes. The sign factors $\hat{Z}_\lambda$ denote whether the corresponding column $S_{mi,\lambda}$ corresponds to a creation or annihilation operator for the collective mode.

Application to a translationally invariant system with a density-density interaction

Density-density interaction in momentum space and in Hartree-Fock basis:



$$= -V(\mathbf{q})\left[\Lambda_{\mathbf{q}}(\mathbf{k})\right]_{\beta\alpha}\left[\Lambda^{\dagger}_{\mathbf{q}}(\mathbf{k}')\right]_{\lambda\sigma}$$

$\left[\Lambda_{\mathbf{q}}(\mathbf{k})\right]_{\beta\alpha} = \langle \mathbf{k}-\mathbf{q},\beta|\mathbf{k},\alpha\rangle$ = Overlaps of cell-periodic part of the HF eigenstates

Collective mode operators: $\sum_{\mathbf{k}}\sum_{\alpha\beta}\phi^{n}_{\mathbf{q},\alpha\beta}(\mathbf{k})c^{\dagger}_{\mathbf{k},\alpha}c_{\mathbf{k}-\mathbf{q},\beta}$ ← n and **q** label the collective mode; α, β and **k** are indices of the wavefunction.

If we define $X^{n}_{\mathbf{q}}(\mathbf{k}) = P^{\perp}(\mathbf{k})\phi^{n}_{\mathbf{q}}(\mathbf{k})P(\mathbf{k}-\mathbf{q})$

$Y^{n}_{\mathbf{q}}(\mathbf{k}) = P(\mathbf{k})\phi^{n}_{\mathbf{q}}(\mathbf{k})P^{\perp}(\mathbf{k}-\mathbf{q})$

Colums of S are labeled by n and **q**

With P the HF projector, and $P^{\perp}$ its complement, then the general equation $S^{\dagger}ZS = \hat{Z}$ becomes

$$\sum_{\mathbf{k}}\left[\mathrm{tr}(X^{n}_{\mathbf{q}}(\mathbf{k})X^{n\dagger}_{\mathbf{q}}(\mathbf{k})) - \mathrm{tr}(Y^{n}_{\mathbf{q}}(\mathbf{k})Y^{n\dagger}_{\mathbf{q}}(\mathbf{k}))\right] = \eta_{\mathbf{q},n} = \pm 1$$

Application to a translationally invariant system with a density-density interaction

The general eigenvalue equation $ZS\hat{Z}\Omega = H_B S$ becomes

Collective mode energies

$$
\begin{aligned}
(n_\alpha(\mathbf{k}) - n_\beta(\mathbf{k}-\mathbf{q}))\phi^n_{\mathbf{q},\alpha\beta}(\mathbf{k})\eta_{\mathbf{q},n}\omega_{\mathbf{q},n} \;=\; & |E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}-\mathbf{q})|\phi^n_{\mathbf{q},\alpha\beta}(\mathbf{k}) \\
& + V(\mathbf{q})\frac{1}{N}\sum_{\mathbf{k}'} \mathrm{tr}\left(\phi^n_{\mathbf{q}}(\mathbf{k}')\Lambda_{\mathbf{q}}(\mathbf{k}')\right)\left[\Lambda^\dagger_{\mathbf{q}}(\mathbf{k})\right]_{\alpha\beta} \\
& - \frac{1}{N}\sum_{\mathbf{q}'} V(\mathbf{q}')\left[\Lambda^\dagger_{\mathbf{q}'}(\mathbf{k})\phi_{\mathbf{q}}(\mathbf{k}-\mathbf{q}')\Lambda_{\mathbf{q}'}(\mathbf{k}-\mathbf{q})\right]_{\alpha\beta},
\end{aligned}
$$

Using the solutions to this equation, the propagator of the nth collective mode can be written as

$$
\left[G^n_2(i\nu,\mathbf{q})\right]_{(\mathbf{k},\alpha\beta);(\mathbf{k}',\lambda\sigma)} = \phi^n_{\mathbf{q},\alpha\beta}(\mathbf{k})\frac{1}{\omega_{\mathbf{q},n} - i\nu\,\eta_{\mathbf{q},n}}\phi^{n*}_{\mathbf{q},\lambda\sigma}(\mathbf{k}')
$$

RPA collective modes = Time-Dependent Hartree-Fock collective modes

The RPA Bethe-Salpeter equation can also be obtained from applying the Time-Dependent Variational Principle (TDVP) with Slater determinants.

$$\mathcal{L}_{TDVP}(\dot{M}, M) = \frac{i}{2}\frac{\langle\psi(\dot{M})|\psi(M)\rangle - \langle\psi(M)|\psi(\dot{M})\rangle}{\langle\psi(M)|\psi(M)\rangle} - \frac{\langle\psi(M)|H|\psi(M)\rangle}{\langle\psi(M)|\psi(M)\rangle}$$

$$|\psi(M)\rangle = \exp\left(\sum_{m,i} M_{mi} c_m^\dagger c_i\right)|\psi_0\rangle$$

Expanding this Lagrangian to second order in M and diagonalizing the quadratic part gives the same collective mode spectrum as that obtained from the RPA Bethe-Salpeter equation. We will not do this calculation here.

More details can be found in the following book: *“Geometry of the time-dependent variational principle in quantum mechanics”*

RPA collective modes = Time-Dependent Hartree-Fock collective modes

TDVP with Slater determinants gives rise to the following TDHF equation:

$$i\partial_t P = [H_{HF}[P], P] \qquad \text{(Dirac, 1930)}$$

TDVP exactly conserves the energy:

$$\dot{E} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{tr}\left(P(T + H_{HF}[P])\right) = 0$$

To convince you of the equivalence of RPA and TDHF, we will work out a simple example where we calculate the linear response charge compressibility in TDHF for the following Hamiltonian:

$$H = \sum_{\mathbf{k}}\sum_{s}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k},s}c_{\mathbf{k},s} + \frac{1}{2N}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{s,s'}V(\mathbf{q})c^{\dagger}_{\mathbf{k}+\mathbf{q},s}c^{\dagger}_{\mathbf{k}'-\mathbf{q},s'}c^{\dagger}_{\mathbf{k}',s'}c_{\mathbf{k},s}$$

We perturb it with $\hat{V} = \sum_{\mathbf{k},\mathbf{q}}\sum_{s}V_{\mathbf{q}}(t)c^{\dagger}_{\mathbf{k}+\mathbf{q},s}c_{\mathbf{k},s}$

RPA collective modes = Time-Dependent Hartree-Fock collective modes

As we are doing linear response, let us write $P = P_0 + P_1(t)$, with P_0 a solution of the SC HF equation.

Taking $V_{\mathbf{q}}(t) = V_{\mathbf{q}}(e^{i\omega t} + e^{-i\omega t})$

$$P_1(t) = P_1 e^{i\omega t} + P_1^\dagger e^{-i\omega t}$$

and working up to first order in both V and P_1, we find the following change in the charge density (also ignoring the exchange term)

$$\delta\langle n_{\mathbf{q}}\rangle = \frac{1}{N}\sum_{\mathbf{k}}\sum_{s}\langle \mathbf{k}, s|P_1|\mathbf{k}+\mathbf{q}, s\rangle = \frac{\Pi(\omega,\mathbf{q})}{1+V(\mathbf{q})\Pi(\omega,\mathbf{q})}V_{\mathbf{q}}$$

with

$$\Pi(\omega,\mathbf{q}) = \frac{2}{N}\sum_{\mathbf{k}}\frac{n(\mathbf{k})-n(\mathbf{k}+\mathbf{q})}{\omega - E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}}}$$

→ Occupation numbers

→ HF mean-field energies of P_0

the standard polarization bubble. We have thus reproduced the RPA result from TDHF. The details are left as an exercise.

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