Correlated electron-phonon systems - exact diagonalization method

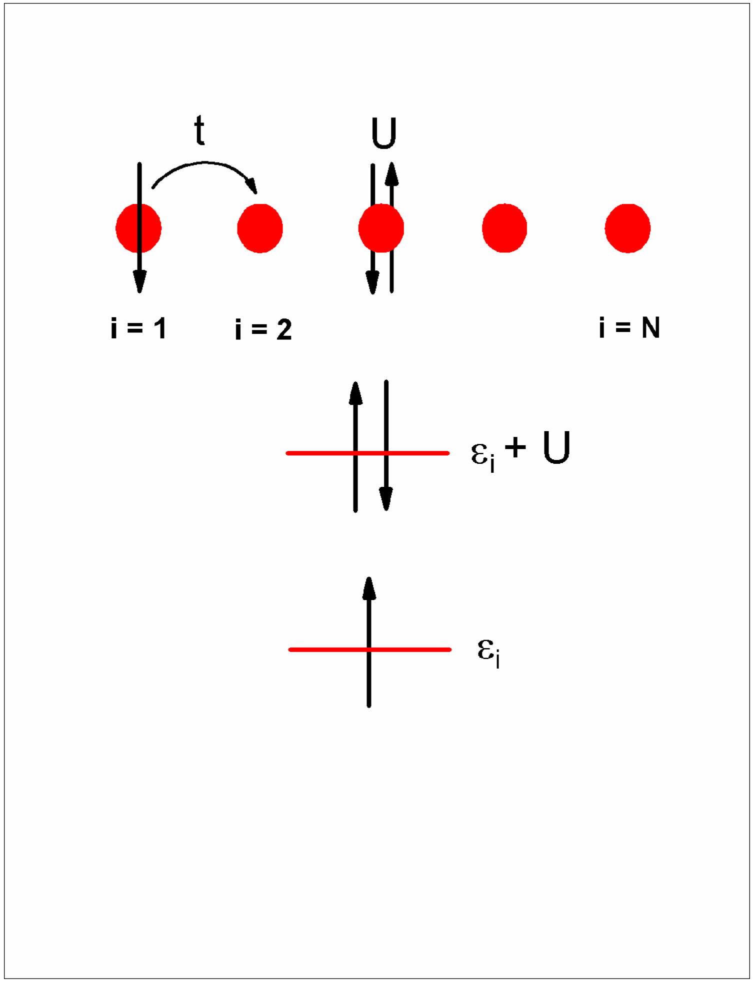
1. Hubbard model
2. Electron-phonon coupling
3. Lanczos method
4. Spectral properties
    a) Phonon renormalization and scattering cross sections
    b) Charge dynamics
    c) Spin dynamics
    d) Optical conductivity

Hubbard model

$$H = \sum_{i=1}^{N} (\varepsilon_i n_i + U_i n_{i,\uparrow} n_{i,\downarrow}) + \sum_{i,j,\sigma=\uparrow,\downarrow} t_{ij} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma})$$

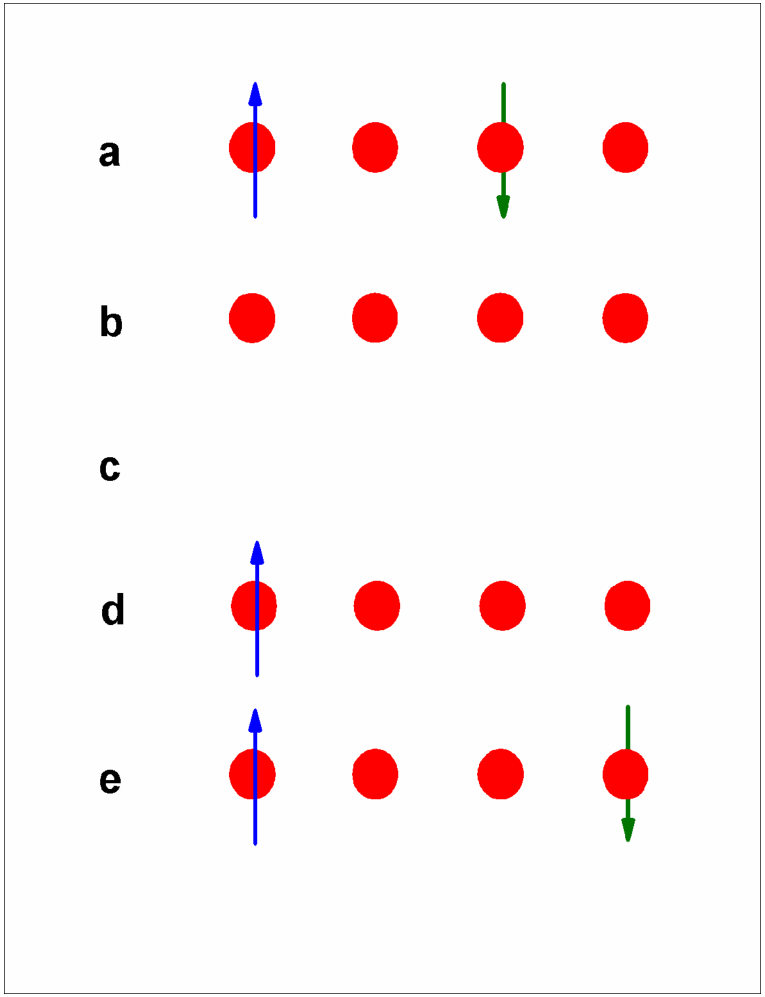
$$n_i = n_{i,\uparrow} + n_{i,\downarrow}$$

$$n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$$



Quantum Field Theory Kindergarten

1. $|0\rangle$
2. $c^\dagger_{1,\uparrow}|0\rangle$
3. $c^\dagger_{1,\uparrow}c^\dagger_{4,\downarrow}|0\rangle$
4. $c_{1,\uparrow}|0\rangle$
5. $c^\dagger_{1,\uparrow}c^\dagger_{1,\uparrow}|0\rangle$
6. $c^\dagger_{1,\uparrow}c_{1,\uparrow}|0\rangle$
7. $c^\dagger_{1,\uparrow}c_{1,\uparrow}|\uparrow,0,0,0\rangle$
8. $c^\dagger_{1,\uparrow}c_{1,\uparrow}|0,\uparrow,0,0\rangle$
9. $c_{1,\downarrow}|\uparrow\downarrow,0,\downarrow,0\rangle$
10. $c^\dagger_{1,\uparrow}c^\dagger_{4,\downarrow}c_{1,\downarrow}c_{4,\downarrow}|\downarrow,0,0,\downarrow\rangle$



$$
\begin{aligned}
\{c_{i,\sigma}, c^\dagger_{j,\sigma'}\} &= c_{i,\sigma}c^\dagger_{j,\sigma'} + c^\dagger_{j,\sigma'}c_{i,\sigma} = \delta_{ij}\delta_{\sigma\sigma'} \\
\{c^\dagger_{i,\sigma}, c^\dagger_{j,\sigma'}\} &= c^\dagger_{i,\sigma}c^\dagger_{j,\sigma'} + c^\dagger_{j,\sigma'}c^\dagger_{i,\sigma} = 0 \\
\{c_{i,\sigma}, c_{j,\sigma'}\} &= c_{i,\sigma}c_{j,\sigma'} + c_{j,\sigma'}c_{i,\sigma} = 0
\end{aligned}
$$

$$|i,\sigma;j,\sigma'\rangle = c^\dagger_{i,\sigma}c^\dagger_{j,\sigma'}|0\rangle = -c^\dagger_{j,\sigma'}c^\dagger_{i,\sigma}|0\rangle = -|j,\sigma';i,\sigma\rangle$$

Pauli exclusion principle

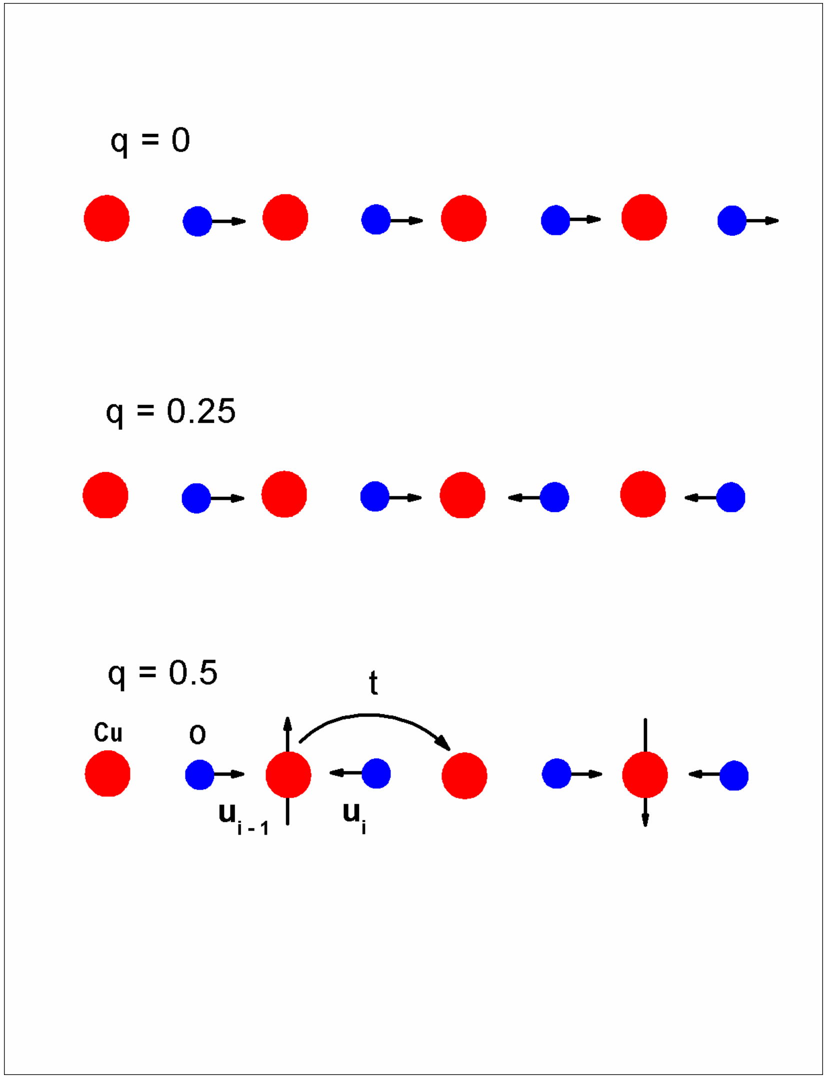
$$c^\dagger_{i,\sigma}c^\dagger_{i,\sigma} = -c^\dagger_{i,\sigma}c^\dagger_{i,\sigma} \rightarrow (c^\dagger_{i,\sigma})^2 = 0$$

Electron-phonon interaction

$$H_p = \frac{m}{2}\sum_{i=1}^{N}(\dot{u}_i^2 + \omega^2 u_i^2)$$

$$H_{e-p} = -\lambda \sum_{i=1}^{N} n_i(u_i - u_{i-1})$$

$$X_q = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} u_i(q) = \frac{1}{\sqrt{N}}\sum_{i=1}^{N} u_i e^{iqr_i}$$



Quantization: creation and annihilation operators

$$X_q = \sqrt{\frac{\hbar}{2m\omega_q}}(b_q^\dagger + b_q) \qquad P_q = i\sqrt{\frac{m\hbar\omega_q}{2}}(b_q^\dagger - b_q)$$

$$[X_{q'}, P_q] = X_{q'}P_q - P_qX_{q'} = i\hbar\delta_{q,q'} \quad \rightarrow \quad [b_{q'}, b_q^\dagger] = \delta_{q,q'}$$

$$[b_{q'}^\dagger, b_q^\dagger] = 0 \qquad [b_{q'}, b_q] = 0$$

$$b_q^\dagger|0\rangle = |1_q\rangle \qquad b_q|0\rangle = 0$$

$$b_q^\dagger|M_q\rangle = \sqrt{M_q+1}|M_q+1\rangle \qquad b_q|M_q\rangle = \sqrt{M_q}|M_q-1\rangle$$

$$\hat{M}_q|M_q\rangle = b_q^\dagger b_q|M_q\rangle = M_q|M_q\rangle$$

Electron-phonon Hamiltonian

$$H = H_e + H_p + H_{e-p}$$

$$H_e = -t\sum_{i,j,\sigma}(c^\dagger_{i,\sigma}c_{j,\sigma} + c^\dagger_{j,\sigma}c_{i,\sigma}) + U\sum_i n_{i,\uparrow}n_{i,\downarrow}$$

$$H_p = \sum_q \hbar\omega_q(b^\dagger_q b_q + \frac{1}{2})$$

$$H_{e-p} = \sum_{i=1,q}^{N} g(q)n_i e^{iqr_i}(b^\dagger_q + b_{-q})$$

$$g(q) = -2i\lambda\sqrt{\frac{\hbar}{2m\omega N}}\sin\left(\frac{q}{2}\right)$$

$$\hbar\omega\alpha = \lambda\sqrt{\frac{\hbar}{2m\omega}}$$

Hilbert space

$$H|\Psi\rangle = E|\Psi\rangle$$

$$|\Psi\rangle = \sum_{\mu=n,M}^{Dim} \alpha_\mu |\mu\rangle \qquad |\mu\rangle = |n\rangle|M\rangle$$

$$|n\rangle = |\uparrow, 0, \downarrow, 0, \uparrow\downarrow, \ldots\rangle \qquad |M\rangle = \prod_q |M_q\rangle$$

$$Dim = Dim_e * Dim_p$$

$$Dim_e = \frac{N!}{(N-N_\uparrow)!N_\uparrow!} * \frac{N!}{(N-N_\downarrow)!N_\downarrow!}$$

$$Dim_p = \infty \simeq 10 - 20$$

$$\sum_{\nu=1}^{Dim} H_{\mu,\nu}\alpha_\nu = E\alpha_\mu \qquad H_{\mu,\nu} = \langle\mu|H|\nu\rangle$$

Example: two-site model

$$H = -\ t(c^\dagger_{1,\uparrow}c_{2,\uparrow} + c^\dagger_{2,\uparrow}c_{1,\uparrow} + c^\dagger_{1,\downarrow}c_{2,\downarrow} + c^\dagger_{2,\downarrow}c_{1,\downarrow})$$
$$+\ U(n_{1,\uparrow}n_{1,\downarrow} + n_{2,\uparrow}n_{2,\downarrow})$$

$\varepsilon_1 = \varepsilon_2 = 0$

$\mathrm{Dim}_e = 4$

$|\,1 > \; = |\uparrow\downarrow, 0 >$

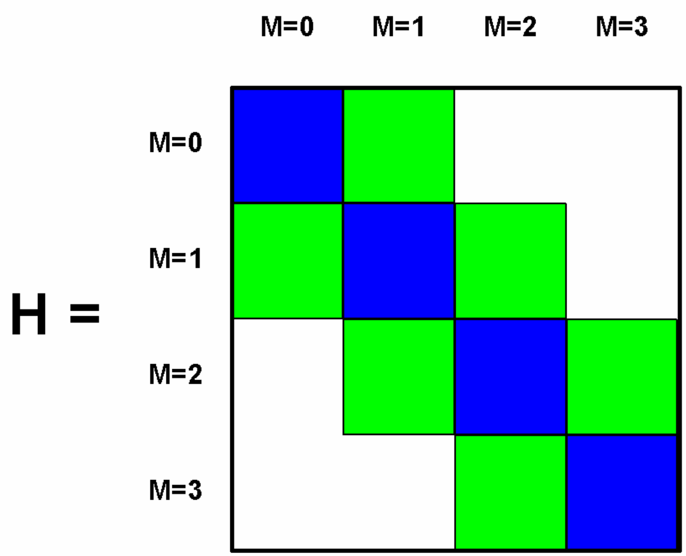
$|\,2 > \; = |\,0, \uparrow\downarrow >$

$|\,3 > \; = |\uparrow, \downarrow >$

$|\,4 > \; = |\downarrow, \uparrow >$

$<1|H|1> = U$
$<2|H|2> = U$
$<3|H|3> = 0$
$<4|H|4> = 0$
$<1|H|2> = 0$
$<1|H|3> = -t$
....

$$\mathbf{H_e} = \begin{vmatrix} U & 0 & -t & -t \\ 0 & U & -t & -t \\ -t & -t & 0 & 0 \\ -t & -t & 0 & 0 \end{vmatrix}$$



$Dim = Dim_e * Dim_p \quad Dim_p = 10\text{-}20$

$N=8 \quad x = 0 \quad Dim_e = 4900$

$N=8 \quad x = 1/4 \quad Dim_e = 3136$

$N=12 \quad x = 1/6 \quad Dim_e = 627264$

Exact diagonalization - Lanczos method

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$|\phi_0\rangle$ - initial random vector

$$|\phi_1\rangle = H|\phi_0\rangle - a_0|\phi_0\rangle$$

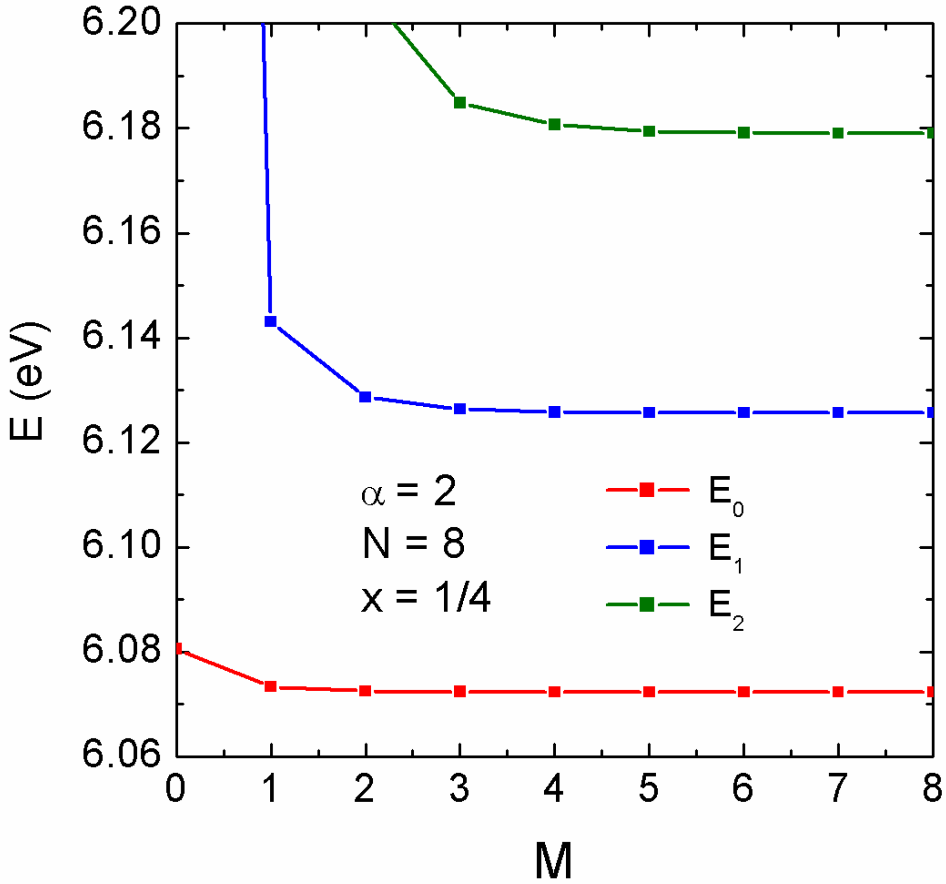
$$|\phi_2\rangle = H|\phi_1\rangle - a_1|\phi_1\rangle - b_1^2|\phi_0\rangle$$

$$|\phi_{m+1}\rangle = H|\phi_m\rangle - a_m|\phi_m\rangle - b_m^2|\phi_{m-1}\rangle$$

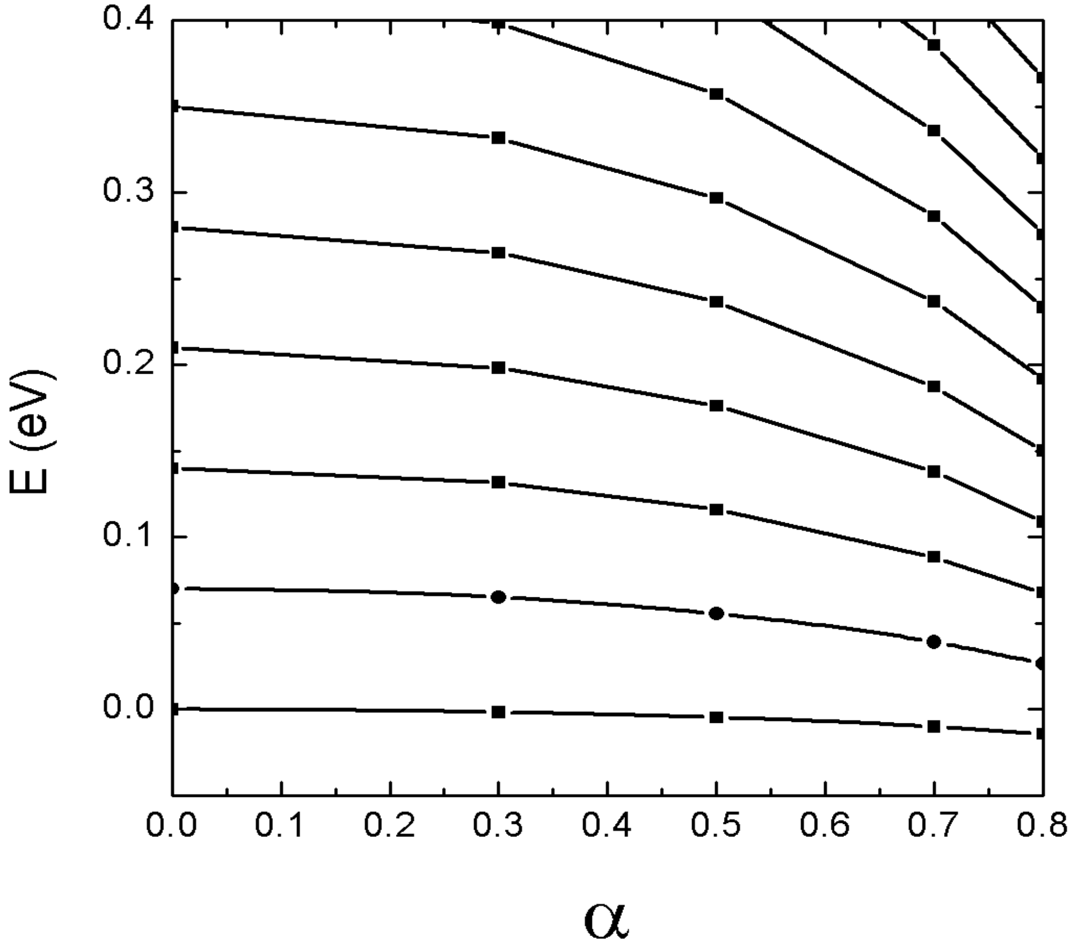
$$a_m = \frac{\langle\phi_m|H|\phi_m\rangle}{\langle\phi_m|\phi_m\rangle} \qquad b_m^2 = \frac{\langle\phi_m|\phi_m\rangle}{\langle\phi_{m-1}|\phi_{m-1}\rangle}$$

$$|\psi_n\rangle = \sum_{m=1}^{L} c_m^n|\phi_m\rangle \qquad L \sim 100$$

$$H = \begin{vmatrix} a_0 & b_1 & 0 & 0 & 0 & \dots \\ b_1 & a_1 & b_2 & 0 & 0 & \dots \\ 0 & b_2 & a_2 & b_3 & 0 & \dots \\ 0 & 0 & b_3 & a_3 & b_4 & \dots \end{vmatrix}$$



6.20
6.18
6.16
6.14
6.12
6.10
6.08
6.06
E (eV)
0
1
2
3
4
5
6
7
8
M
α = 2
N = 8
x = 1/4
E0
E1
E2



0.4
0.3
0.2
0.1
0.0
E (eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
α