APPLICATION OF CONTINUOUS UNITARY TRANSFORMATIONS TO IONIC HUBBARD MODEL

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Outline

Introduction to CUT Method

Ionic Hubbard Model

Flow Equations for IHM

Summary and Conclusions

Introduction to CUT Method

- ***Eigenvalues, eigenvectors and correlation functions of a quantum system***
- ***Diagonalization using continuous unitary transformation***

$$H = H^d + H^r$$

- ***Transformed Hamiltonian***

$$H(\ell) = U(\ell) H U^\dagger(\ell)$$

- ***Flow equations***: Define a **Generator** $\eta(\ell)$

$$\frac{dH(\ell)}{dl} = [\eta(\ell), H(\ell)], \quad U(\ell) = e^{\eta(\ell)}$$

The generator governs the flow, and hence determines in which sector the Hamiltonian renormalizes itself

- ***Wegner Generator***: Quantum fluctuations driven flow

$$H(\ell) = H^d(\ell) + H^r(\ell)$$

$$\eta(\ell) = [H(\ell), H^r(\ell)],$$

- ***Wegner Generator*** $\Rightarrow$ ***Block Diagonalization***

$$\ell \to \infty : \quad h_{ab}(\infty)\left(h_{aa}(\infty) - h_{bb}(\infty)\right) = 0$$

Band Matrices

A matrix is called band matrix, *iff*

$$H_{nm} = 0; \qquad \text{for } |n-m| > M$$

MKU (Mielke, Knetter, Uhrig) generator

$$\eta_{ij}(\ell) = sgn(q_i(\ell) - q_j(\ell))H_{ij}(\ell)$$

where Q is an operator counting number of some kind of excitations, allows for "particle number conserving" flow.

- η^{MKU} ***preservs band nature***

PROOF

$$\frac{dh_{nm}}{d\ell} = -sgn(n-m)(h_{nn}-h_{mm})h_{nm} + \sum_{k\neq n,m}[sgn(n-k)+sgn(m-k)]h_{nk}h_{km}$$

- First term $\propto \hat{h} \Rightarrow$ Band matrix
- For $|n-m| > M$ either of k_{nk} or h_{km} is zero
- For $m \leq k \leq n$, $\sum_k$ over *sgn*'s with different sing $\Rightarrow$ zero
- For $k \notin [m,n]$, *sgn*'s add up to ± 2

$$+2 \sum_{m-M<k<m} h_{nk}h_{km} - 2 \sum_{n<k<M} h_{nk}h_{km}$$

Example: Two-level Hamiltonian

$$H = E\mathbf{1} - \frac{\omega}{2}\sigma^z + \frac{e}{2}\sigma^x$$

Using $Q = (\mathbf{1} - \sigma^z)/2$ one takes $H_d = E\mathbf{1} - \frac{\omega}{2}\sigma^z$, to obtain $\eta_{11} = \eta_{22} = 0$, $\eta_{12} = sgn(0-1)e/2$, $\eta_{21} = sgn(1-0)e/2$, which can be summarized as $\eta = -ie/2\sigma^y$. Hence:

$$\partial_\ell H = -\frac{ie}{2}[\sigma^y, E\mathbf{1} - \frac{\omega}{2}\sigma^z + \frac{e}{2}\sigma^x] = \frac{ie\omega}{2} i\sigma^x + \frac{ie^2}{2} i\sigma^z \Rightarrow$$

$$\partial_\ell \begin{pmatrix} E - \omega/2 & e/2 \\ e/2 & E + \omega/2 \end{pmatrix} = -\frac{e}{2} \begin{pmatrix} e & \omega \\ \omega & -e \end{pmatrix} \Rightarrow$$

$$\partial_\ell E = 0, \quad \partial_\ell \omega = e^2, \quad \partial_\ell e = -\omega e \Rightarrow$$

$$E^{(\infty)} = E, \quad \omega^{(\infty)} = \sqrt{\omega^2 + e^2}, \quad e^{(\infty)} = 0$$

Exercise

Repeat the previous procedure with the bosonic oscillator

$$H = E\mathbf{1} + \omega a^\dagger a + \frac{d}{2}\left(a^{\dagger 2} + a^2\right)$$

Hint: Take $Q = a^\dagger a$ to obtain $\eta = \frac{d}{2}(a^{\dagger 2} - a^2)$

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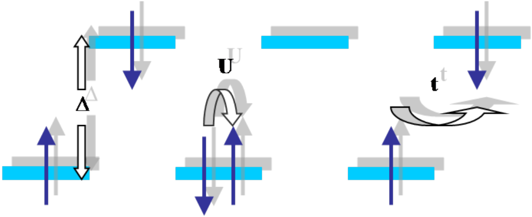
Ionic Hubbard Model

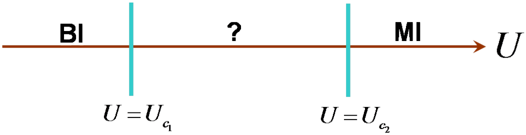
- ***Motivation***:
  - Neutral-ionic transition in organic compounds
  - Ferroelectric transition in perovskite materials.
- ***Ionic Hubbard Hamiltonian***:

$$H = -t \sum_{\langle j,l \rangle} \sum_{\sigma} \left(c^{\dagger}_{j\sigma} c_{l\sigma} + c^{\dagger}_{l\sigma} c_{j\sigma} \right) + U \sum_{j} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} + \frac{\Delta}{2} \sum_{i,\sigma} (-1)^{i} c^{\dagger}_{i\sigma} c_{i\sigma}$$



Ionic Hubbard Model

- Definition of the problem:



What is the state of the system between Mott and band insulators?

- ***Ionic Hubbard model in the limit*** $\mathbf{U = 0}$:

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} \varepsilon_{k+\pi}\, c^\dagger_{k+\pi\sigma} c_{k+\pi\sigma} + \frac{\Delta}{2} \sum_{k\sigma} (c^\dagger_{k\sigma} c_{k+\pi\sigma} + h.c.)$$

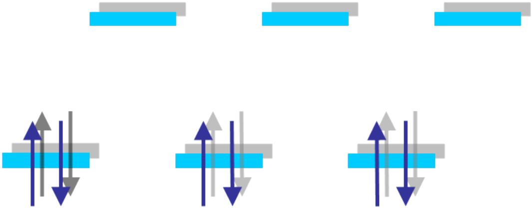
Where $\varepsilon_k = -2t\cos k$. Using Bogolubov transformations:

$$H = \sum_{k\sigma} E_k \left(\gamma^\dagger_{k\sigma}\gamma_{k\sigma} - \gamma^\dagger_{k+\pi\sigma}\gamma_{k+\pi\sigma}\right)$$

Where:

$$E_k = \sqrt{4t^2\cos^2 k + (\frac{\Delta}{2})^2}$$

Ionic Hubbard Model



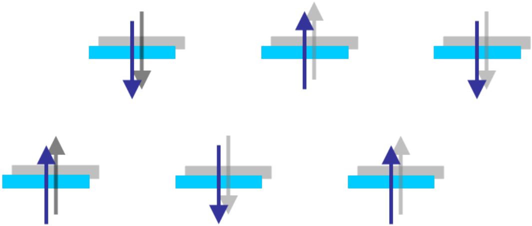
Therefore in half-filling conditions IHM is band insulator With energy gap Δ.

- ***Ionic Hubbard model in the limit*** $U \gg t$:

Reduces to t-J model which at half-filling describes a Mott insulator

- Frozen charge fluctuations at half-filling
- Low-energy spin-exciations

$$H = J \sum_{\langle i,j \rangle} \vec{S}_i . \vec{S}_{i+1}, \quad J = \frac{4t^2}{U} \tag{0}$$

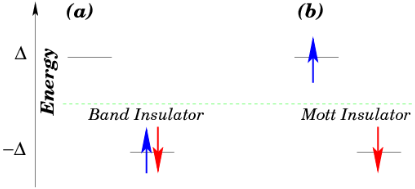


Another solvable limit: Classic Limit

- ***Atomic limit*** ($\mathbf{t} = \mathbf{0}$):

$$H = U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} + \frac{\Delta}{2} \sum_{i,\sigma} (-1)^i \, \hat{n}_{i,\sigma} \qquad (0)$$

In this limit IHM is classical and line $U = \Delta$ separates band insulator from Mott insulator.



The line $U = \Delta$ is metallic transition point.

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Warm up exercise

- ***Flow equations for IHM in the limit*** $\mathbf{U = 0}$:

Split $H_0(\ell)$ as:

$$H_0(\ell) = \sum_{k\sigma} \varepsilon_k(\ell)\, c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} \varepsilon_{k+\pi}(\ell)\, c^\dagger_{k+\pi\sigma} c_{k+\pi\sigma} + \sum_{k,\sigma} \frac{\Delta_k(\ell)}{2} (c^\dagger_{k\sigma} c_{k+\pi\sigma} + h.c.)$$

Wegner generator becomes:

$$\eta_0(\ell) = \sum_{k,\sigma} \frac{\Delta_k(\ell)}{2} \left(\varepsilon_k(\ell) - \varepsilon_{k+\pi}(\ell)\right) \left(c^\dagger_{k\sigma} c_{k+\pi\sigma} - h.c.\right)$$

Flow Equation

$$[\eta_0(\ell), H_0(\ell)] =$$
$$-\sum_{k,\sigma} \frac{\Delta_k(\ell)}{2} \left(\varepsilon_k(\ell) - \varepsilon_{k+\pi}(\ell)\right)^2 \left(c^\dagger_{k\sigma} c_{k+\pi\sigma} + h.c.\right)$$
$$+\sum_{k,\sigma} \frac{\Delta_k^2(\ell)}{2} \left(\varepsilon_k(\ell) - \varepsilon_{k+\pi}(\ell)\right) \left(c^\dagger_{k,\sigma} c_{k,\sigma} - c^\dagger_{k+\pi\sigma} c_{k+\pi\sigma}\right)$$

Which gives the following flow equations:

$$\frac{d\varepsilon_k(\ell)}{d\ell} = \Delta_k^2(\ell)\,\varepsilon_k(\ell)$$
$$\frac{d\Delta_k(\ell)}{d\ell} = -4\Delta_k(\ell)\,\varepsilon_k^2(\ell)$$
$$\varepsilon_k(\ell) = -\varepsilon_{k+\pi}(\ell)$$

Solution of flow equations

In the limit $\ell \to \infty$

$$\Delta_k(\infty) = 0$$

$$\varepsilon_k(\infty) = \pm\sqrt{\left(\frac{\Delta}{2}\right)^2 + 4\,t^2\cos^2 k} \quad \begin{cases} + & k \in (-\frac{\pi}{2}, 0] \\ - & k \in (-\pi, \frac{\pi}{2}] \end{cases}$$

- **Result is identical to Bogolubov transformation.**

Flow Equations for IHM

- ***Effective Hamiltonian For IHM***

$H(\ell)$ is considered as:

$$H(\ell) = -t(\ell)\sum_{i\sigma}\left(c^{\dagger}_{i,\sigma}c_{i+1\sigma} + h.c.\right) + \frac{\Delta(\ell)}{2}\sum_{i\sigma}(-1)^{i}c^{\dagger}_{i\sigma}c_{i\sigma}$$

$$+\frac{U(\ell)}{2}\sum_{i\sigma\sigma'}c^{\dagger}_{i\sigma}c^{\dagger}_{i\sigma'}c_{i\sigma'}c_{i\sigma} + V(\ell)\sum_{i\sigma\sigma'}c^{\dagger}_{i\sigma}c^{\dagger}_{i+1\sigma'}c_{i+1\sigma'}c_{i\sigma}$$

With initial conditions $t(0) = 1$, $\Delta(0) = \Delta$, $U(0) = U$, and $V(0) = 0$

Wegner generator for IHM

$$\eta(\ell) = t(\ell)\,\Delta(\ell)\sum_{i,\sigma}(-1)^i\left(c^\dagger_{i+1,\sigma}c_{i,\sigma} - h.c.\right)$$
$$-t(\ell)\,U(\ell)\sum_{i,\sigma\sigma'}\left(c^\dagger_{i,\sigma}c^\dagger_{i,\sigma'}c_{i,\sigma'}c_{i+1,\sigma} - c^\dagger_{i-1,\sigma}c^\dagger_{i,\sigma'}c_{i,\sigma'}c_{i,\sigma} - h.c.\right)$$
$$-t(\ell)\,V(\ell)\sum_{i,\sigma\sigma'}\left(c^\dagger_{i,\sigma}c^\dagger_{i+1,\sigma'}c_{i+1,\sigma'}c_{i+1,\sigma} + c^\dagger_{i,\sigma}c^\dagger_{i+1,\sigma'}c_{i+2,\sigma'}c_{i,\sigma}\right.$$
$$\left.- c^\dagger_{i,\sigma}c^\dagger_{i,\sigma'}c_{i+1,\sigma'}c_{i,\sigma} - c^\dagger_{i-1,\sigma}c^\dagger_{i+1,\sigma'}c_{i+1,\sigma'}c_{i,\sigma} - h.c.\right)$$

Some Algebra

With definitions: $\eta(\ell) \equiv \eta_1(\ell) + \eta_2(\ell) + \eta_3(\ell)$
$H(\ell) = H_1(\ell) + H_2(\ell) + H_3(\ell) + H_4(\ell)$
Various commutators can be calculated:

$$[\eta(\ell), H_1(\ell) + H_2(\ell)] =$$
$$2t^2(\ell)\Delta(\ell)\sum_{i,\sigma}(-1)^i\left(c^\dagger_{i,\sigma}c_{i,\sigma} + c^\dagger_{i,\sigma}c_{i+2,\sigma} + h.c.\right)$$
$$+t(\ell)\Delta^2(\ell)\sum_{i,\sigma}\left(c^\dagger_{i+1,\sigma}c_{i,\sigma} + h.c.\right)$$
$$[\eta_2(\ell), H_1(\ell)] = 2t^2(\ell)U(\ell)\sum_{i,\sigma\sigma'}\left(c^\dagger_{i,\sigma}c^\dagger_{i,\sigma'}c_{i,\sigma'}c_{i,\sigma}\right.$$
$$\left.-c^\dagger_{i+1,\sigma}c^\dagger_{i,\sigma'}c_{i,\sigma'}c_{i+1,\sigma} + h.c.\right) + \textit{irrelevant terms}$$

Some More Algebra

$$[\eta_3(\ell), H_1(\ell)] = 2t^2(\ell)\, V(\ell) \sum_{i,\sigma\sigma'} \Big(2c^\dagger_{i,\sigma} c^\dagger_{i+1,\sigma'} c_{i+1,\sigma'} c_{i,\sigma} - c^\dagger_{i,\sigma} c^\dagger_{i,\sigma'} c_{i,\sigma'} c_{i,\sigma} + h.c. \Big) + \textit{irrelevant terms}$$

Differential Equations

$$\frac{dt(\ell)}{d\ell} = -t(\ell)\,\Delta^2(\ell)$$
$$\frac{d\Delta(\ell)}{d\ell} = 8t^2(\ell)\,\Delta(\ell)$$
$$\frac{dU(\ell)}{d\ell} = 8t^2(\ell)\,(U(\ell) - V(\ell))$$
$$\frac{dV(\ell)}{d\ell} = 4t^2(\ell)\,(2V(\ell) - U(\ell))$$

- Hopping term flows to zero!
- Quantum fluctuations are being renormalized to zero
- Attractive longer reange Coulomb interaction induced

Solutions at $\ell \to \infty$:

$$t(\infty) = 0$$

$$\Delta(\infty) = \left(8+\Delta^2\right)^{\frac{1}{2}}$$

$$U(\infty) = \frac{U}{2}\frac{\left(8+\Delta^2\right)^{\frac{1}{2}}\left(\left(8+\Delta^2\right)^{\frac{\sqrt{2}}{4}}+\left(8+\Delta^2\right)^{-\frac{\sqrt{2}}{4}}\Delta^{\sqrt{2}}\right)}{\Delta^{1+\frac{\sqrt{2}}{2}}}$$

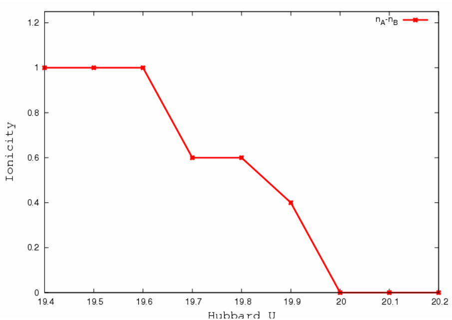
$$V(\infty) = \frac{\sqrt{2}U}{4}\frac{\left(8+\Delta^2\right)^{\frac{1}{2}}\left(-\left(8+\Delta^2\right)^{\frac{\sqrt{2}}{4}}+\left(8+\Delta^2\right)^{-\frac{\sqrt{2}}{4}}\Delta^{\sqrt{2}}\right)}{\Delta^{1+\frac{\sqrt{2}}{2}}}$$

Renormalized "Classical" Hamiltonian:

$$H_{eff} \equiv H(\infty) = \frac{\Delta(\infty)}{2}\sum_{i\sigma}(-1)^i\hat{n}_{i\sigma} + U(\infty)\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + V(\infty)\sum_{i\sigma\sigma'}\hat{n}_{i\sigma}\hat{n}_{i+1\sigma'}$$

IONICITY

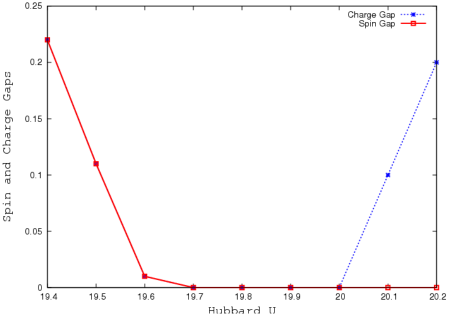
$$n_B = \frac{1}{N}\sum_{\sigma,i\in\mathrm{B}} \langle \widehat{n}_{i\sigma} \rangle, \quad n_A = \frac{1}{N}\sum_{\sigma,i\in\mathrm{A}} \langle \widehat{n}_{i\sigma} \rangle$$



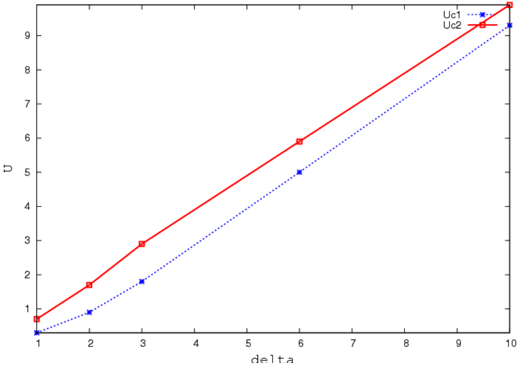
Definitions of spin and charge gaps

- ***Phase Transitions***

$$\Delta_s = E_0\left(\frac{N}{2}+1, \frac{N}{2}-1\right) - E_0\left(\frac{N}{2}, \frac{N}{2}\right)$$
$$\Delta_c = \frac{1}{2}\left(E_0\left(\frac{N}{2}+1, \frac{N}{2}+1\right) + E_0\left(\frac{N}{2}-1, \frac{N}{2}-1\right) - 2E_0\left(\frac{N}{2}, \frac{N}{2}\right)\right)$$



Phase Diagram



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For a fixed Δ

- At small U, both charge and spin gaps are identical
- In the intermediate region, charge gap vanishes $\Rightarrow$ Metallic region
- For large U, charge gap develops once more $\Rightarrow$ Insulator
- Low energy spin-excitations $\Rightarrow$ Mott Insulator

- Faculty position @ IUT physics
  Applications should be addressed to:
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  Head of the physics department,
  Isfahan University of Technology,
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  Fax: 0311-391 2376
  email: shirani@cc.iut.ac.ir
- Thank you for your attention

Example 2: Electron-Phonon Interactions

- Aim: replacement of electron-phonon interaction with an electron-electron interaction:
- Main Hamiltonian:

$$H = \sum_q \omega_q : a_q^\dagger a_q : + \sum_k \varepsilon_k : c_k^\dagger c_k : + \sum_{k,q} M_q \left(a_{-q}^\dagger + a_q \right) c_{k+q}^\dagger c_k + E \equiv H_0 + H_{e-p}(1)$$

- Review on Fröhlich methods:

$$H^F = e^{-S} H e^S = H + [H, S] + \frac{1}{2} [[H, S], S] + \cdots$$

Flow Equations for Electron-Phonon Interactions

$$
\begin{aligned}
H^F &= \sum_{k,k',q} V^F_{k,k',q} : c^\dagger_{k+q} c^\dagger_{k'-q} c_{k'} c_k : \\
&+ \sum_k \left(\varepsilon^F_k - 2 \sum_q n_{k+q} V_{k,k+q,q} \right) : c^\dagger_k c_k : \\
&+ \sum_q \omega^F_q : a^\dagger_q a_q : + E^F + \textit{irrelevant terms} \qquad (2)
\end{aligned}
$$

Flow Equations for Electron-Phonon Interactions

- Flow equations approach:

$H(\ell)$ is approximated as:

$$\begin{aligned} H(\ell) &= E(\ell) + \sum_q \omega_q(\ell) : a_q^\dagger a_q : \\ &+ \sum_k \left(\varepsilon_k(\ell) - 2 \sum_q n_{k+q} V_{k,k+q,q}(\ell) \right) : c_k^\dagger c_k : \\ &+ \sum_{k,k',q} V_{k,k',q}(\ell) : c_{k+q}^\dagger c_{k'-q}^\dagger c_{k'} c_k : \\ &+ \sum_{k,q} \left(M_{k,q}(\ell) a_{-q}^\dagger + M_{k+q,-q}^*(\ell) a_q \right) c_{k+q}^\dagger c_k \qquad (3) \end{aligned}$$

Last term is off-diagonal and other terms are diagonal.

Flow Equations for Electron-Phonon Interactions

Flow equations are obtained as:

$$\frac{dM_{k,q}(\ell)}{d\ell} = -\alpha^2_{k,q}(\ell) M_{k,q}(\ell)$$

$$\begin{aligned}\frac{dV_{k,k',q}(\ell)}{d\ell} &= M_{k,q}(\ell) M^*_{k'-q,q}(\ell) \beta_{k',-q}(\ell) \\ &\quad -M_{k',-q}(\ell) M^*_{k+q,-q}(\ell) \alpha_{k',-q}(\ell)\end{aligned} \tag{4}$$

$$\frac{d\varepsilon_k(\ell)}{d\ell} = -2\sum_q \Big((n_q+1)\left|M_{k,q}(\ell)\right|^2 \alpha_{k,q}(\ell) + n_q \left|M_{k+q,-q}(\ell)\right|^2 \beta_{k,q}($$

$$\frac{d\omega_q(\ell)}{d\ell} = 2\sum_k \left|M_{k+q,-q}(\ell)\right|^2 \beta_{k,q}(\ell) \left(n_{k+q} - n_k\right)$$

Flow Equations for Electron-Phonon Interactions

$$\frac{dE(\ell)}{d\ell} = \sum_k n_k \frac{d\varepsilon_k(\ell)}{d\ell} - \sum_{k,q} n_k n_{k+q} \frac{dV_{k,k+q,q}(\ell)}{d\ell}$$

Where $\alpha_{k,q}(\ell) = \varepsilon_{k+q}(\ell) - \varepsilon_k(\ell) + \omega_q(\ell)$ and $\beta_{k,q}(\ell) = \varepsilon_{k+q}(\ell) - \varepsilon_k(\ell) - \omega_q(\ell)$ are defined.
Solutions in infinity:
$\varepsilon_k(\infty) = \varepsilon_k^F$, $E(\infty) = E^F$, $\omega_q(\infty) = \omega_q^F$ and

$$V_{k,k',q}(\infty) = |M_q|^2 \left(\frac{\beta_{k',-q}}{\alpha_{k,q}^2 + \beta_{k',-q}^2} - \frac{\alpha_{k',-q}}{\alpha_{k',-q}^2 + \beta_{k,q}^2} \right)$$

$$V_{k,k',q}^F = V_{k,-k,q}^F = |M_q|^2 \frac{\omega_q}{(\varepsilon_{k+q} - \varepsilon_k)^2 - \omega_q^2}$$