Anomalous propagators and the particle-particle correlation channel

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The one-body Green function

$$G(11') = (-\mathrm{i}) \langle \Psi_0^N | \hat{T}[\hat{\psi}(1)\hat{\psi}^\dagger(1')] | \Psi_0^N \rangle$$

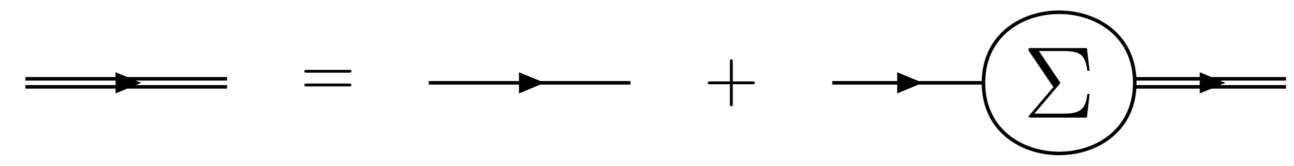
$$G(\mathbf{x}_1\mathbf{x}_{1'};\omega) = \sum_S \frac{\mathcal{I}_S(\mathbf{x}_1)\mathcal{I}_S^*(\mathbf{x}_{1'})}{\omega - (E_0^N - E_S^{N-1}) - \mathrm{i}\eta} + \sum_S \frac{\mathcal{A}_S(\mathbf{x}_1)\mathcal{A}_S^*(\mathbf{x}_{1'})}{\omega - (E_S^{N+1} - E_0^N) + \mathrm{i}\eta}$$

S-th ionization potentials — S-th electron affinities

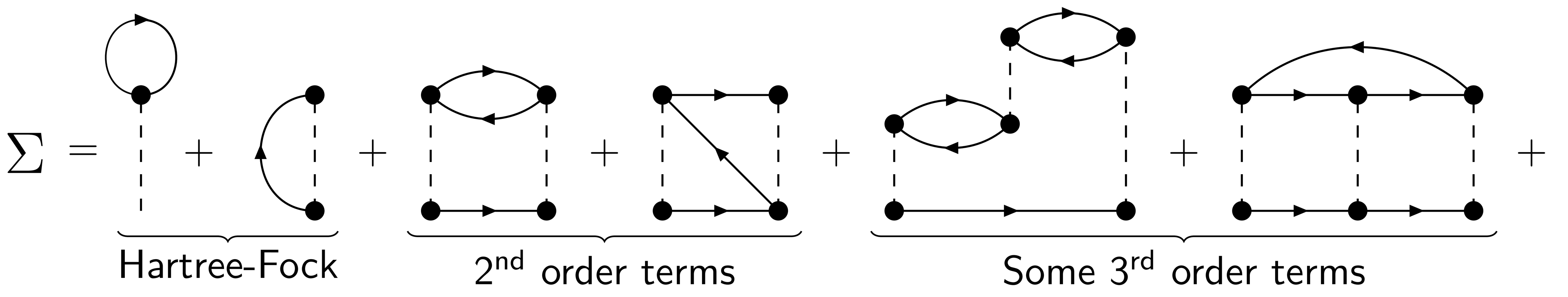
The Dyson equation

$$G(11') = G_0(11') + \int \mathrm{d}(22')\, G_0(12)\Sigma(22')G(2'1')$$

Self-energy



Exact self-energy expansion



Hedin's equations

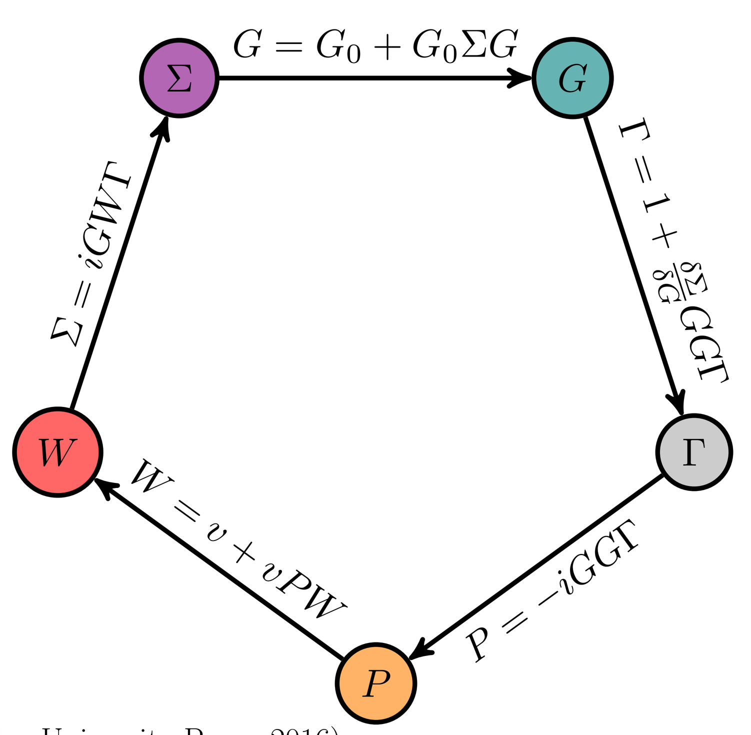
$$G(11') = G_0(11') + G_0(12)\Sigma(22')G(2'1')$$

$$\Sigma_{\mathrm{xc}}(11') = \mathrm{i}G(33')W(12';32)\tilde{\Gamma}(3'2;1'2')$$

$$W(12;1'2') = v(12^-;1'2') - \mathrm{i}W(14;1'4')\tilde{L}(3'4';3^+4)v(23;2'3')$$

$$\tilde{L}(12;1'2') = G(13)G(3'1')\tilde{\Gamma}(32;3'2')$$

$$\tilde{\Gamma}(12;1'2') = \delta(12')\delta(1'2) + \frac{\delta\Sigma_{\mathrm{xc}}(11')}{\delta G(33')}G(34)G(4'3')\tilde{\Gamma}(42;4'2')$$



L. Hedin, Phys. Rev. 139, A796 (1965); R. M. Martin, L. Reining, and D. M. Ceperley, (Cambridge University Press, 2016)

Particle-particle Hedin's equations

$$G(11') = G_0(11') + G_0(12)\Sigma(22')G(2'1')$$

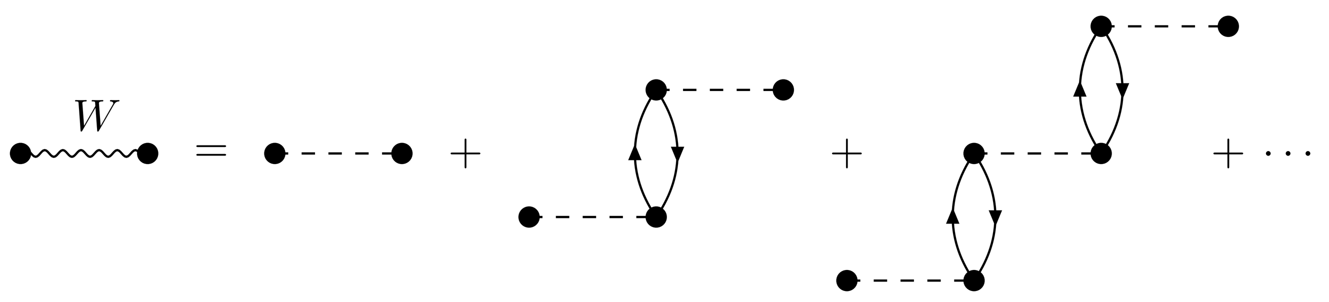
$$\Sigma(11') = \mathrm{i}G(2'2^{++})T(12;33')\tilde{\Gamma}(33';2'1')$$

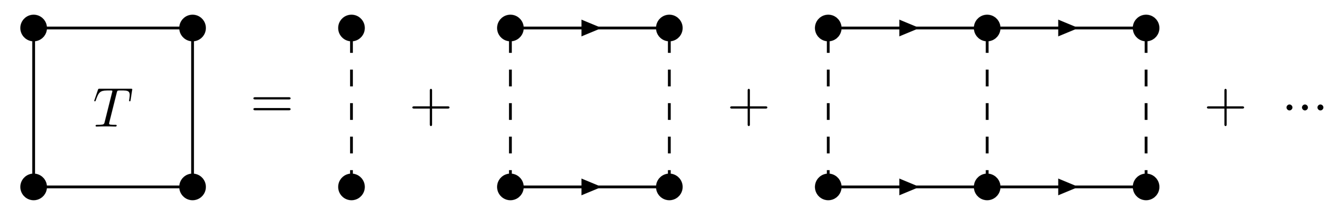
$$T(12;1'2') = -\bar{v}(12;1'2') - T(12;33')\tilde{K}(33';44')v(44'^+;1'2'^{++})$$

$$\tilde{K}(12;1'2') = \mathrm{i}G(31')G(3'2')\tilde{\Gamma}(12;33')$$

$$\tilde{\Gamma}(12;1'2') = \frac{1}{2}[\delta(1'2)\delta(2'1) - \delta(1'1)\delta(2'2)] - \left.\frac{\delta\Sigma^{\mathrm{ee}}(1'2')}{\delta G^{\mathrm{ee}}(33')}\right|_{U=0} G(43)G(4'3')\tilde{\Gamma}(12;44')$$

Effective interactions





External potential and linear response

$$\hat{\mathcal{U}}^{\mathrm{eh}}(t_2) = \int \mathrm{d}(\mathbf{x}_2\mathbf{x}_{2'})\, \hat{\psi}^\dagger(\mathbf{x}_2)U^{\mathrm{eh}}(\mathbf{x}_2\mathbf{x}_{2'};t_2)\hat{\psi}(\mathbf{x}_{2'}) \quad \Rightarrow G_2(12;1'2') = -\left.\frac{\delta G(11')}{\delta U^{\mathrm{eh}}(2'2)}\right|_{U=0} + G(11')G(22')$$

$$\hat{\mathcal{U}}^{\mathrm{pp}}(t_2) = \frac{1}{2}\int \mathrm{d}(\mathbf{x}_2\mathbf{x}_{2'}) \left[\begin{array}{l} \hat{\psi}^\dagger(\mathbf{x}_2)U^{\mathrm{ee}}(\mathbf{x}_2\mathbf{x}_{2'};t_2)\hat{\psi}^\dagger(\mathbf{x}_{2'}) \\ + \hat{\psi}(\mathbf{x}_2)U^{\mathrm{hh}}(\mathbf{x}_2\mathbf{x}_{2'};t_2)\hat{\psi}(\mathbf{x}_{2'}) \end{array} \right] \quad \Rightarrow G_2(12;1'2') = -2\left.\frac{\delta G^{\mathrm{ee}}(1'2')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0}$$

Gorkov propagator

$$\boldsymbol{G}(11') = (-i)\langle \Psi_0 | \hat{T}\left[\begin{pmatrix} \hat{\psi}(1)\hat{\psi}^\dagger(1') & \hat{\psi}(1)\hat{\psi}(1') \\ \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1') & \hat{\psi}^\dagger(1)\hat{\psi}(1') \end{pmatrix} \right] | \Psi_0 \rangle$$

$$= \begin{pmatrix} G^{\mathrm{he}}(11') & G^{\mathrm{hh}}(11') \\ G^{\mathrm{ee}}(11') & G^{\mathrm{eh}}(11') \end{pmatrix}$$

L. P. Gorkov, Sov. Phys. JETP 34, 505 (1958)

Particle-particle Bethe-Salpeter equation

$$K(12;1'2') = \frac{1}{2}(G(21')G(12') - G(11')G(22')) - \int \mathrm{d}(34)\, K(12;44')\Xi^{\mathrm{pp}}(44';33')K_0(33';1'2')$$

$$\int \mathrm{d}(3'44')\, G(24)\Xi^{\mathrm{pp}}(34;3'4')K(3'4';1'2') = \int \mathrm{d}(3'44')\, G(41')\left.\frac{\delta\Sigma(34)}{\delta G(3'4')}\right|_{U=0} L(3'2;4'2')$$

$$\Xi^{\mathrm{pp}}(12;34) = \left.\frac{\delta\Sigma^{\mathrm{ee}}(34)}{\delta G^{\mathrm{ee}}(12)}\right|_{U=0}$$

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