lowing general real-space Dyson equation (for a time-invariant system),

$$G_{ij,\sigma}(\omega) = G^0_{ij,\sigma}(\omega) + \sum_{kl} G^0_{ik,\sigma}(\omega)\Sigma_{kl,\sigma}(\omega)G_{lj,\sigma}(\omega)\,. \tag{1.26}$$

This is also the defining equation for the proper self-energy.[18] For translationally invariant systems one can simplify this equation by Fourier transformation,

$$G^{-1}_\sigma(\boldsymbol{k},\omega) = (G^0_\sigma(\boldsymbol{k},\omega))^{-1} - \Sigma(\boldsymbol{k},\omega); \quad \Sigma(\boldsymbol{k},\omega) \equiv \Sigma(\omega)\;. \tag{1.27}$$

Consequently, the local Green function can be expressed in terms of the noninteracting DOS and the self-energy alone,

$$G_\sigma(\omega) \equiv G_{ii,\sigma}(\omega) = \frac{1}{V_B}\sum_{\boldsymbol{k}} \frac{1}{\omega+\mu-\epsilon_{\boldsymbol{k}}-\Sigma_\sigma(\omega)} \tag{1.28}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}\epsilon \frac{\rho(\epsilon)}{\omega+\mu-\epsilon-\Sigma_\sigma(\omega)}\;. \tag{1.29}$$

An alternative derivation of the $\boldsymbol{q}$-independence of the proper self-energy is based on the observation that the Laue function $\delta^*(\boldsymbol{q}) = \sum_{\boldsymbol{K}} \delta(\boldsymbol{q}+\boldsymbol{K})$ (with reciprocal lattice vectors $\boldsymbol{K}$) becomes effectively momentum-independent when applied to the internal vertices of a diagram (such as a vertex of the inserted proper self-energy). Thus, the self-energy cannot depend on the external momentum and is consequently momentum-independent (Müller-Hartmann, 1989*a*).

The absence of momentum dependence in the self-energy greatly simplifies the treatment of the Hubbard model. One may, in fact, single out one of the lattice sites and replace the influence of its neighbors by the interaction with a single, frequency-dependent bath, i.e., map the Hubbard model onto a single impurity Anderson model (SIAM) in the limit $Z \to \infty$. In order to restore the periodicity of the original lattice, this medium has to be determined self-consistently (Jarrell, 1992; Georges and Kotliar, 1992; Janiš and Vollhardt, 1992; Georges, Kotliar, Krauth, and Rozenberg, 1996). Written in terms of fermionic Matsubara frequencies[19] $\omega_n = (2n+1)\pi T$, self-energy $\Sigma_{\sigma n} \equiv \Sigma_\sigma(i\omega_n)$, and Green function $G_{\sigma n} \equiv G_\sigma(i\omega_n)$ the resulting coupled equations read

$$\boxed{\begin{aligned} G_{\sigma n} &= \int_{-\infty}^{\infty} \mathrm{d}\varepsilon\, \frac{\rho(\varepsilon)}{i\omega_n+\mu-\Sigma_{\sigma n}-\varepsilon} && (1.30)\\ G_{\sigma n} &= -\langle \psi_{\sigma n}\psi^*_{\sigma n}\rangle_{\mathcal{A}}. && (1.31) \end{aligned}}$$

[18] A self-energy is called proper if its external vertices cannot be be separated by cutting a single Green function line which implies that they are connected by at least three such lines.

[19] We here chose an imaginary-time formulation for brevity and in anticipation of its use in the context of the imaginary-time quantum Monte Carlo algorithm discussed in Sec. 1.3.