Appendix B Single particle in a non-local potential

The exchange (Fock) term in the single-particle Hartree–Fock equation is non-local in the position coordinate \vec{r} (see Fig. B.1, see also Fig. A1(4)). A short range non-locality can be approximated by a momentum dependence which can be included in the Schrödinger equation by defining a *k*-effective mass m_k . This *k*-mass approximation was introduced in Chapter 8. The effective interaction between nucleons due to phonon exchange has a time dependence, which can be incorporated in an ω -effective mass m_{ω} (Chapter 9). The purpose of this appendix is to discuss some of the properties of these effective masses.

Let us start with the time-dependent Hartree-Fock equation

$$i\hbar \frac{\partial \varphi_{\nu}(\vec{r},t)}{\partial t} = \left(-\frac{\hbar^2 \nabla^2}{2m} + U(r)\right) \varphi_{\nu}(\vec{r},t) + \int d^3 r' U_x(\vec{r},\vec{r}') \varphi_{\nu}(\vec{r}',t), \qquad (B.1)$$

where $U_x(\vec{r}, \vec{r}')$ is the Fock term in the single-particle potential. Let us assume an infinite system and $U(r) = V_0$ (constant) for simplicity. Consequently,

$$\varphi_{\nu}(\vec{r},t) = e^{i(\vec{k}_{\nu}\cdot\vec{r}-\omega t)}/\sqrt{V}, \qquad (B.2)$$

where V is the volume of the system.

Replacing this wavefunction in equation (B.1) leads to

$$\begin{split} \hbar \omega \mathrm{e}^{\mathrm{i}(\vec{k}_{v}\cdot\vec{r}-\omega t)} &= \left(\frac{\hbar^{2}k_{v}^{2}}{2m} + V_{0}\right)\mathrm{e}^{\mathrm{i}(\vec{k}_{v}\cdot\vec{r}-\omega t)} \\ &+ \int \mathrm{d}^{3}r' \, U_{x}(\vec{r},\vec{r}\,')\mathrm{e}^{\mathrm{i}(\vec{k}_{v}\cdot\vec{r}'-\omega t)} \end{split}$$

Multiplying from the left by $e^{-i(\vec{k}_v \cdot \vec{r} - \omega t)}$ and making use of the fact that $U_x(\vec{r}, \vec{r}')$ does not depend on the centre of mass coordinate $\vec{R} = (\vec{r} + \vec{r}')/2$ but only on the relative coordinate $\rho = \vec{r} - \vec{r}'$ and that the Jacobian $\partial(\vec{\rho}, \vec{R})/\partial(\vec{r}, \vec{r}') = 1$, one obtains

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + V_0 + U_x(k). \tag{B.3}$$

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Figure B.1. Coupling of a particle to a vibration (left). Exchange diagram associated with the Fock potential (right).

Here $\varepsilon = \hbar \omega$ is the single-particle energy and

$$U_x(k) = \int \frac{\mathrm{d}^3 R}{V} \int \mathrm{d}^3 \varrho \mathrm{e}^{-\mathrm{i}(\vec{k_\nu}.\vec{r}-\omega t)} U_x(\vec{r},\vec{r}\,') \mathrm{e}^{\mathrm{i}(\vec{k_\nu}.\vec{r}\,'-\omega t)}$$
$$= \int \mathrm{d}^3 \varrho \mathrm{e}^{-\mathrm{i}\vec{k_\nu}.\vec{\varrho}} U_x(\vec{r},\vec{r}\,')$$

is the Fourier transform of the Fock (exchange) potential. Let us force an independent single-particle dispersion relation by absorbing the non-local potential in an effective k-mass

$$\varepsilon = \frac{\hbar^2 k^2}{2m_k} + \tilde{V}_0, \tag{B.4}$$

where \tilde{V}_0 is a constant. From the relation (note that we are determining an inertia, i.e. studying the reaction of the system to a change in its state of motion)

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}k} = \frac{\hbar^2 k}{m} + \frac{\partial U_x}{\partial k} \approx \frac{\hbar^2 k}{m_k},\tag{B.5}$$

which assumes that m_k is approximately constant, we obtain

$$m_k = m \left(1 + \frac{m}{\hbar^2 k} \frac{\partial U_x}{\partial k} \right)^{-1}.$$
 (B.6)

The momentum dependence in equation (B.3) can be replaced by a dispersion relation for the energy

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + U(\varepsilon). \tag{B.7}$$

From equation (B.4) one can write

$$\frac{\hbar^2 k^2}{2m} = \frac{m_k}{m} \left(\varepsilon - \tilde{V}_0\right).$$

Replacing this relation in equation (B.7) one obtains

$$U(\varepsilon) = \varepsilon - \frac{m_k}{m} \left(\varepsilon - \tilde{V}_0 \right)$$
$$= \frac{m_k}{m} \tilde{V}_0 + \left(1 - \frac{m_k}{m} \right) \varepsilon.$$
(B.8)

Inserting this relation in equation (B.7) and comparing with equation (B.3) one obtains

$$V_0 = \frac{m_k}{m} \tilde{V}_0$$

Summing up

$$\varepsilon = \frac{\hbar^2 k^2}{2m_k} + \frac{m}{m_k} V_0. \tag{B.9}$$

In other words, equations (B.3) and (B.9) should provide an equivalent description of the system under consideration. Note that m_k may depend on r.

B.1 Single particle in a non-local, ω -dependent potential

The processes depicted in Fig. B.1 give rise to a non-local (*k*-dependent) and timedependent (ω -dependent) potential. In what follows we shall discuss some of its consequences making use of a one-dimensional system. Equation (B.1) becomes

$$i\hbar \frac{\partial \varphi_{\nu}(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \varphi_{\nu}(x,t) + \int dx' \, dt' \, U(x'-x,t'-t) \, \varphi_{\nu}(x',t') \,. \tag{B.10}$$

Making use of wavefunctions like the one given in equation (B.2), but in one dimension, one obtains

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + \int \mathrm{d}x' \,\mathrm{d}t' \,\mathrm{e}^{\mathrm{i}(k(x'-x)-\omega(t'-t))} U(x'-x,t'-t),$$

leading to

$$\hbar\omega = \varepsilon = \frac{\hbar^2 k^2}{2m} + V_0 + U(k,\omega), \qquad (B.11)$$

where $U(k, \omega)$ is the Fourier transform of U(x' - x, t' - t). Again, we impose the singleparticle dispersion relation introducing an effective mass m^* , i.e.

$$\hbar\omega = \frac{\hbar^2 k^2}{2m^*} + \tilde{V}^0.$$
(B.12)

Taking the derivative of equation (B.11) with respect to k one obtains

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}k} \left(1 - \frac{\partial U}{\partial \varepsilon} \right) = \frac{\hbar^2 k}{m} \left(1 + \frac{m}{\hbar^2 k} \frac{\partial U}{\partial k} \right). \tag{B.13}$$

We now make the approximation

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}k} = \frac{\hbar^2 k}{m^*}.\tag{B.14}$$

One can interpret the left-hand side of this equation as the rate of change in energy when the momentum changes or, equivalently, when the number of nodes per unit length changes. Since the latter can be used to label the single-particle states, the energy spacing between levels, i.e. the density of levels, changes as m^* changes. Note that this statement also applies to equation (B.5). Note also that m_w may depend on r.

Inserting the relation (B.14) in equation (B.13) one obtains

$$\frac{m^*}{m} = \frac{m_\omega}{m} \frac{m_k}{m},\tag{B.15}$$

where

$$\frac{m_{\omega}}{m} = \left(1 - \frac{\partial U}{\partial(\hbar\omega)}\right) \tag{B.16}$$

and

$$\frac{m_k}{m} = \left(1 + \frac{m}{\hbar^2 k} \frac{\partial U}{\partial k}\right)^{-1}.$$
(B.17)

Assuming a dispersion relation of the form (B.7) for the energy we get

$$U(\varepsilon) = \frac{m^*}{m}\tilde{V}^0 + \left(1 - \frac{m^*}{m}\right)\varepsilon.$$
(B.18)

From the comparison of equations (B.7) and (B.8) with equation (B.11) one obtains

$$\widetilde{V}^0 = \frac{m}{m^*} V^0.$$

Summing up

$$\varepsilon = \frac{\hbar k^2}{2m^*} + \frac{m}{m^*} V_0. \tag{B.19}$$

To bridge the gap between infinite nuclear matter and the case of potential wells of finite range let us consider a particle of mass m in a one-dimensional harmonic potential (see Mahaux (1985)). The Hamiltonian describing its motion,

$$H = \frac{p^2}{2m} + \frac{C}{2}x^2,$$
 (B.20)

leads to discrete energy levels with a constant spacing

$$\hbar\omega_0 = \hbar \sqrt{\frac{C}{m}}.$$
(B.21)

It follows from this expression that the density of states is proportional to the square root of m. We notice, however, that this result is derived by assuming that the potential remains unchanged if the bare mass is replaced by an effective mass. If this is the case, the ground-state wavefunction

$$\Psi_0 \sim \exp\left(-\frac{x^2}{2b^2}\right) \tag{B.22}$$

with

$$b = \sqrt{\frac{\hbar^2}{mC}} \tag{B.23}$$

for a particle of mass $m^* > m$ will shrink in space compared with the one of mass *m* and consequently the mean square radius of the system

$$\langle r^2 \rangle = \frac{\hbar}{m^* \omega_0} \left(N + \frac{3}{2} \right) = b^2 \left(N + \frac{3}{2} \right) \tag{B.24}$$

will decrease. This is of course not correct, and one has to impose the condition $b^2 =$ constant. This condition implies that the energy difference between levels is inversely proportional to the mass (or effective mass) of the system, in keeping with the fact that

$$\hbar\omega_0 = \frac{\hbar^2}{m^* b^2},\tag{B.25}$$

see equations (B.5) and (B.14), as well as the discussion following equation (9.9).

Because the inverse of the level distance at the Fermi energy is proportional to the density of levels $\rho(\varepsilon_{\rm F})$ (see Eq. (2.1)), $\rho(\varepsilon_{\rm F}) \sim m^*$. Within this context, one can interpret the left-hand side of Eq. (B.14) as the rate of change in energy when the momentum changes or, equivalently, when the number of nodes per unit length changes. Since the latter can be used to label the single-particle states, the energy spacing between levels decreases for increasing values of m^* . Thus, the density of single-particle levels at the Fermi energy is proportional to the effective mass. (To be noted that while $\rho(\varepsilon_{\rm F}) = 3A/2\varepsilon_{\rm F} (\varepsilon_{\rm F} = \hbar^2 k_{\rm F}^2/2m^*)$ is the total density of single-particle levels (i.e. spin-up and -down and both protons and neutrons), $\rho(\varepsilon_{\rm F})/4$ is the level density associated with a single spin orientation and with one type of nucleon (either protons or neutrons).)

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